IUCrData

ISSN 2414-3146

4-Bromo-2-[({2-[(2-hydroxyethyl)amino]ethyl}-imino)methyl]phenol

Erika Samoľová,[a]* Aliakbar Dehno Khalaji[b] and Václav Eigner[a]

[a]Institute of Physics AS CR, v.v.i., Na Slovance 2, 182 21 Prague 8, Czech Republic, and [b]Department of Chemistry, Faculty of Science, Golestan University, Gorgan, Iran. *Correspondence e-mail: samolova@fzu.cz

Received 23 March 2021
Accepted 29 March 2021

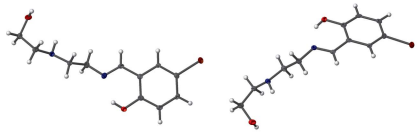
Edited by M. Bolte, Goethe-Universität Frankfurt, Germany

Keywords: crystal structure; Schiff base; hydrogen bonds.

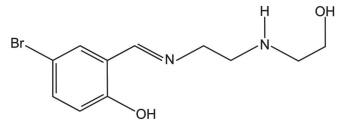
Structural data: full structural data are available from iucrdata.iucr.org

The new title Schiff base compound, $C_{11}H_{15}BrN_2O_2$, crystallizes in the monoclinic space group $P2_1$ with two independent molecules in the asymmetric unit. It was prepared by the condensation reaction of 5-bromo-2-hydroxybenzaldehyde and aminoethylethanolamine. There is an intramolecular O—H···N hydrogen bond with an $S(6)$ ring motif. Moreover, there are intermolecular C—H···N, C—H···O and Br···O interactions in the crystal structure of the title compound.

3D view



Chemical scheme



Structure description

Schiff bases and their derivatives have played a key role in the development of coordination chemistry (Vafazadeh *et al.*, 2019; Ghorbani *et al.*, 2017) due to their easy preparation, structural diversity, biological properties, catalytic activity and also their ability to act as chelating ligands (Böhme & Fels, 2020; Adrian *et al.*, 2020; Saranya *et al.*, 2020; Yousif *et al.*, 2017; Guo *et al.*, 2019; Bhattacharjee *et al.*, 2017; Shweta *et al.*, 2016; Reimann *et al.*, 2019; Ceylan *et al.*, 2015; Salehi *et al.*, 2016; Zhu *et al.*, 2019; Kumar *et al.*, 2019; Atahan & Durmus, 2015). In the present work, we report the crystal structure of the new Schiff base, commonly known as aminoethylethanolamine-5-bromo-2-hydroxybenzaldehyde. The asymmetric unit of the title compound contains two independent molecules, as shown in Fig. 1. All bond lengths and angles are within their expected ranges according to other published Schiff base structures (Böhme & Fels, 2020; Ceylan *et al.*, 2015; Salehi *et al.*, 2016). The N1*a*=C7*a* double bond is 1.273 (6) Å and N1*b*=C7*b* 1.276 (7) Å, the N1*a*—C8*a* single bond is 1.460 (6) Å and N1*b*—C8*b* 1.455 (7) Å, in good agreement with the corresponding values for the similar compounds (Salehi *et al.*, 2016; Ceylan *et al.*, 2015). The bond angles C7*a*—N1*a*—C8*a* [118.0 (4)°], C7*b*—N1*b*—C8*b* [117.9 (4)°], C2*a*—C7*a*—N1*a* [121.5 (4)°] and C2*b*—C7*b*—N1*b* [121.7 (4)°] are also in agreement with those angles in the similar compounds (Salehi *et al.*, 2016; Ceylan *et al.*,

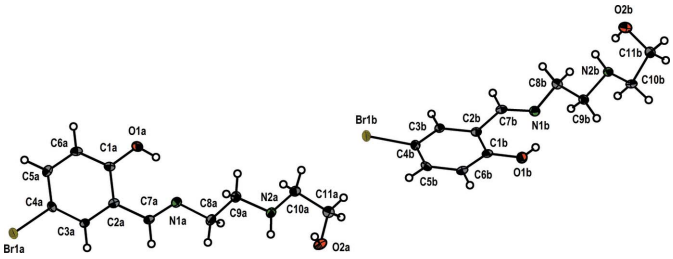


Figure 1
The asymmetric unit of the title structure. Displacement ellipsoids are drawn at the 50% probability level.

2015). An intramolecular hydrogen bond with an $S(6)$ ring is observed in each independent molecule. Moreover, the O2*a* and O2*b* atoms are involved in a second intramolecular hydrogen bond. The molecules are connected through intermolecular O—H···N hydrogen bonds and Br···O interactions with distances Br1*a*···O2*b* = 3.206 (2) Å and Br1*b*···O2*a* = 3.282 (2) Å (Fig. 2, Table 1).

Synthesis and crystallization

5-Bromo-2-hydroxybenzaldehyde (2 mmol) was dissolved in ethanol (10 ml) and stirred for 10 min. Then, a solution of aminoethylethanolamine (0.2 mmol) dissolved in ethanol (5 ml) was added dropwise. The mixture was stirred and refluxed for 6 h. After that, the solution was concentrated under reduced pressure. Yellow crystals suitable for X-ray analysis were obtained by slow evaporation of solvent at room temperature for several days. These were filtered off and washed several times with cold ethanol.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Marching Cube ELD software (MCS) was used for the electron density map visualization (Rohlíček & Hušák, 2007).

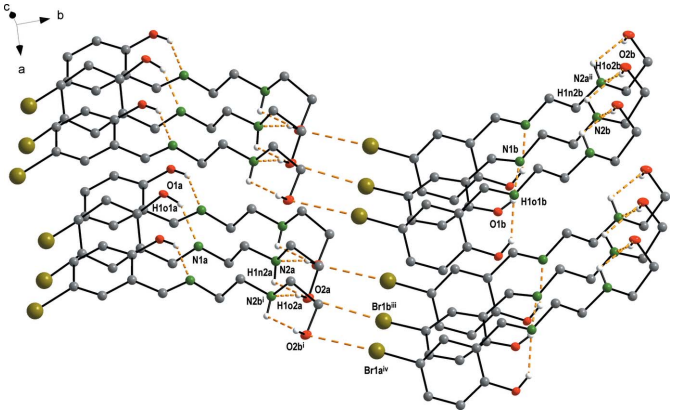


Figure 2
View of the hydrogen-bond system and the Br···O interactions in the title compound. Hydrogen atoms not involved in hydrogen bonding are omitted for clarity. Symmetry codes: (i) $2-x, y-\frac{1}{2}, 2-z$; (ii) $1-x, \frac{1}{2}+y, 1-z$; (iii) $1+x, y, z$; (iv) $3-x, \frac{1}{2}+y, 2-z$.

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

D—H···A	D—H	H···A	D···A	D—H···A
O1*a*—H1*o*1*a*···N1*a*	0.82 (5)	1.89 (6)	2.597 (5)	144 (5)
O2*a*—H1*o*2*a*···N2*b*^{i}	0.82 (3)	2.02 (4)	2.826 (6)	168 (6)
O1*b*—H1*o*1*b*···N1*b*	0.82 (5)	1.91 (6)	2.587 (6)	139 (5)
O2*b*—H1*o*2*b*···N2*a*^{ii}	0.82 (3)	2.06 (4)	2.859 (6)	165 (6)
N2*a*—H1*n*2*a*···O2*a*	0.88 (3)	2.45 (5)	2.871 (6)	110 (5)
N2*b*—H1*n*2*b*···O2*b*	0.88 (3)	2.44 (5)	2.884 (5)	112 (5)

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{11}H_{15}BrN_2O_2$
M_r	287.2
Crystal system, space group	Monoclinic, $P2_1$
Temperature (K)	95
a, b, c (Å)	6.0518 (2), 27.7837 (7), 6.9028 (2)
β (°)	90.497 (2)
V (Å^3)	1160.60 (6)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	4.74
Crystal size (mm)	0.38 × 0.25 × 0.04
Data collection	
Diffractometer	Rigaku Oxford Diffraction SuperNova, Dual, Cu at zero, AtlasS2
Absorption correction	Analytical (*CrysAlis PRO*; Rigaku OD, 2015)
T_{min}, T_{max}	0.34, 0.816
No. of measured, independent and observed [$I > 3\sigma(I)$] reflections	8118, 4637, 4488
R_{int}	0.021
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.628
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.055, 0.134, 2.31
No. of reflections	4637
No. of parameters	308
No. of restraints	6
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.81, −0.48
Absolute structure	Flack (1983), 2215 Friedel pairs
Absolute structure parameter	−0.03 (3)

Computer programs: *CrysAlis PRO* (Rigaku OD, 2015), *SUPERFLIP* (Palatinus & Chapuis, (2007), *JANA2006* (Petříček *et al.*, 2014), *MCE* (Rohlíček & Hušák, 2007) and *DIAMOND* (Brandenburg, 1999).

Acknowledgements

The authors are grateful to Golestan University. CzechNanoLab project LM2018110 funded by MEYS CR is gratefully acknowledged for financial support of the measurements at LNSM Research Infrastructure.

References

Adrian, R. A., Canales, D. & Arman, H. D. (2020). *IUCrData*, **5**, x201344.
Atahan, A. & Durmus, S. (2015). *Spectrochim. Acta A*, **144**, 61–67.
Bhattacharjee, A., Halder, S., Ghosh, K., Rizzoli, C. & Roy, P. (2017). *New J. Chem.* **41**, 5696–5706.
Böhme, U. & Fels, S. (2020). *IUCrData*, **5**, x201384.

Brandenburg, K. (1999). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Ceylan, U., Durgun, M., Türkmen, H., Yalçın, P., Kilic, A. & Özdemir, N. (2015). *J. Mol. Struct.* **1089**, 222–232.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Ghorbani, M., Khalaji, A. D., Feizi, N., Akbari, A., Eigner, V. & Dusek, M. (2017). *J. Mol. Struct.* **1130**, 442–446.
Guo, Y., Hu, X., Zhang, X., Pu, X. & Wang, Y. (2019). *RSC Adv.* **9**, 41737–41744.
Kumar, V., Kumar, P., Kumar, S., Singhal, D. & Gupta, R. (2019). *Inorg. Chem.* **58**, 10364–10376.
Palatinus, L. & Chapuis, G. (2007). *J. Appl. Cryst.* **40**, 786–790.
Petříček, V., Dušek, M. & Palatinus, L. (2014). *Z. Kristallogr.***229**, 345–352.
Reimann, M. J., Salmon, D. R., Horton, J. T., Gier, E. C. & Jefferies, L. R. (2019). *ACS Omega*, **4**, 2874–2882.
Rigaku OD (2015). *CrysAlis PRO*. Rigaku Oxford Diffraction, Yarnton, England.
Rohlíček, J. & Hušák, M. (2007). *J. Appl. Cryst.* **40**, 600–601.
Salehi, M., Ghasemi, F., Kubicki, M., Asadi, A., Behzad, M., Ghasemi, M. H. & Gholizadeh, A. (2016). *Inorg. Chim. Acta*, **453**, 238–246.
Saranya, J., Jone Kirubavathy, S., Chitra, S., Zarrouk, A., Kalpana, K., Lavanya, K. & Ravikiran, B. (2020). *Arab. J. Sci. Eng*. **45**, s4683–s4695.
Shweta, S., Neeraj, N., Asthana, S. K., Mishra, R. K. & Upadhyay, K. K. (2016). *RSC Adv.* **6**, 55430–55437.
Vafazadeh,R., Kazemi-nasab, A. & Willis, A.C. (2019). *Acta Chim. Slov*. **66**, 1010–1018.
Yousif, E., Majeed, A., Al-Sammarrae, K., Salih, N., Salimon, J. & Abdullah, B. (2017). *Arabian J. Chem.* **10**, S1639–S1644.
Zhu, X., Duan, Y., Li, P., Fan, H., Han, T. & Huang, X. (2019). *Anal. Methods*, **11**, 642–647.

full crystallographic data

IUCrData (2021). **6**, x210335 [https://doi.org/10.1107/S2414314621003357]

4-Bromo-2-[({2-[(2-hydroxyethyl)amino]ethyl}imino)methyl]phenol

Erika Samoľová, Aliakbar Dehno Khalaji and Václav Eigner

4-Bromo-2-[({2-[(2-hydroxyethyl)amino]ethyl}imino)methyl]phenol

Crystal data

$C_{11}H_{15}BrN_2O_2$
M_r = 287.2
Monoclinic, $P2_1$
Hall symbol: P 2yb
a = 6.0518 (2) Å
b = 27.7837 (7) Å
c = 6.9028 (2) Å
β = 90.497 (2)°
V = 1160.60 (6) Å^3
Z = 4
$F(000)$ = 584
D_x = 1.643 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54184 Å
Cell parameters from 5986 reflections
θ = 6.4–75.4°
μ = 4.74 mm^{-1}
T = 95 K
Platelet, colourless
0.38 × 0.25 × 0.04 mm

Data collection

Rigaku Oxford Diffraction SuperNova, Dual, Cu at zero, AtlasS2 diffractometer
Radiation source: X-ray tube
Mirror monochromator
Detector resolution: 5.2027 pixels mm^{-1}
ω scans
Absorption correction: analytical (CrysAlisPro; Rigaku OD, 2015)
T_{min} = 0.34, T_{max} = 0.816
8118 measured reflections
4637 independent reflections
4488 reflections with $I > 3\sigma(I)$
R_{int} = 0.021
θ_{max} = 75.5°, θ_{min} = 6.4°
h = −7→7
k = −34→34
l = −7→8

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.134
S = 2.31
4637 reflections
308 parameters
6 restraints
103 constraints
H atoms treated by a mixture of independent and constrained refinement
Weighting scheme based on measured s.u.'s $w = 1/(\sigma^2(I) + 0.0016I^2)$
$(\Delta/\sigma)_{max}$ = 0.0004
$\Delta\rho_{max}$ = 0.81 e Å^{-3}
$\Delta\rho_{min}$ = −0.48 e Å^{-3}
Absolute structure: Flack (1983), 2215 Friedel pairs
Absolute structure parameter: −0.03 (3)

Special details

Refinement. All hydrogen atoms were discernible in difference Fourier maps and could be refined to reasonable geometry. Marching Cube ELD software (MCS) was used for the electron density map visualization (Rohlicek & Husak, 2007). According to common practice, H atoms bonded to C were kept in ideal positions with C–H = 0.96 Å while positions of H atom bonded to N and O were refined with restrained bond lengths 0.820 (1) Å for O—H bonds and 0.880 (1) Å for N—H bonds. In both cases U_{iso}(H) was set to 1.2U_{eq}(C,*N*,*O*). All non-hydrogen atoms were refined using harmonic refinement.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Br1a	0.82327 (7)	0.119124 (17)	0.59379 (6)	0.01689 (14)
Br1b	0.67219 (7)	0.617268 (17)	0.82063 (6)	0.01663 (14)
O1a	0.3912 (6)	0.31366 (13)	0.6749 (5)	0.0160 (10)
O2a	1.4292 (6)	0.51220 (14)	0.8603 (5)	0.0181 (10)
O1b	1.0984 (6)	0.81041 (13)	0.9575 (6)	0.0170 (10)
O2b	0.0585 (6)	1.01653 (14)	0.6475 (5)	0.0173 (10)
N1a	0.7625 (7)	0.35173 (15)	0.5676 (6)	0.0136 (11)
N2a	1.0395 (7)	0.46689 (15)	0.7058 (6)	0.0138 (11)
N1b	0.7210 (7)	0.84968 (16)	0.8774 (6)	0.0147 (11)
N2b	0.4536 (7)	0.96878 (15)	0.7831 (6)	0.0130 (11)
C1a	0.4889 (8)	0.27034 (18)	0.6505 (7)	0.0123 (13)
C2a	0.7071 (8)	0.26658 (17)	0.5792 (6)	0.0113 (12)
C3a	0.8022 (7)	0.22102 (17)	0.5563 (7)	0.0110 (12)
C4a	0.6828 (8)	0.18042 (17)	0.6059 (7)	0.0127 (13)
C5a	0.4692 (8)	0.18358 (18)	0.6760 (7)	0.0135 (13)
C6a	0.3746 (8)	0.22869 (18)	0.6977 (7)	0.0136 (13)
C7a	0.8414 (8)	0.30963 (18)	0.5459 (7)	0.0119 (12)
C8a	0.9119 (8)	0.39261 (18)	0.5457 (8)	0.0153 (14)
C9a	0.9002 (8)	0.42429 (17)	0.7262 (7)	0.0156 (13)
C10a	1.0340 (9)	0.49712 (19)	0.8800 (7)	0.0147 (14)
C11a	1.2178 (9)	0.53440 (19)	0.8765 (8)	0.0169 (14)
C1b	1.0028 (8)	0.76776 (19)	0.9183 (7)	0.0132 (13)
C2b	0.7840 (8)	0.76505 (17)	0.8468 (7)	0.0123 (13)
C3b	0.6901 (7)	0.71945 (18)	0.8096 (6)	0.0111 (12)
C4b	0.8125 (8)	0.67826 (17)	0.8475 (7)	0.0128 (13)
C5b	1.0266 (8)	0.68081 (17)	0.9183 (7)	0.0129 (13)
C6b	1.1215 (8)	0.72560 (19)	0.9527 (7)	0.0138 (13)
C7b	0.6447 (8)	0.80791 (19)	0.8387 (7)	0.0131 (13)
C8b	0.5641 (8)	0.8890 (2)	0.8969 (7)	0.0174 (15)
C9b	0.5974 (8)	0.92782 (17)	0.7427 (7)	0.0132 (12)
C10b	0.4570 (8)	1.00481 (18)	0.6268 (7)	0.0140 (14)
C11b	0.2681 (8)	1.04018 (18)	0.6529 (8)	0.0166 (14)
H1o1a	0.477 (9)	0.3360 (17)	0.656 (10)	0.0192*
H1o2a	1.447 (12)	0.501 (2)	0.970 (4)	0.0217*
H1o1b	1.022 (10)	0.8341 (15)	0.933 (10)	0.0204*
H1o2b	0.047 (12)	1.006 (2)	0.537 (4)	0.0208*
H1n2a	1.177 (3)	0.460 (2)	0.679 (9)	0.0165*

H1n2b	0.316 (4)	0.958 (2)	0.786 (9)	0.0157*
H1c3a	0.949114	0.217962	0.506473	0.0132*
H1c5a	0.388396	0.155044	0.708997	0.0162*
H1c6a	0.226862	0.231176	0.746291	0.0163*
H1c7a	0.992328	0.305995	0.506916	0.0142*
H1c8a	0.868714	0.41104	0.433975	0.0184*
H2c8a	1.06028	0.381103	0.530093	0.0184*
H1c9a	0.750008	0.434045	0.7466	0.0187*
H2c9a	0.947685	0.406141	0.837289	0.0187*
H1c10a	1.050579	0.477245	0.992939	0.0176*
H2c10a	0.893641	0.513099	0.887122	0.0176*
H1c11a	1.194585	0.555849	0.769179	0.0203*
H2c11a	1.213354	0.553276	0.992845	0.0203*
H1c3b	0.542552	0.716952	0.758373	0.0133*
H1c5b	1.108922	0.65191	0.943463	0.0155*
H1c6b	1.270528	0.727504	1.00081	0.0166*
H1c7b	0.491711	0.804593	0.8034	0.0157*
H1c8b	0.579114	0.903103	1.023326	0.0208*
H2c8b	0.41626	0.876651	0.887421	0.0208*
H1c9b	0.748732	0.938194	0.744645	0.0159*
H2c9b	0.561579	0.91489	0.617336	0.0159*
H1c10b	0.441354	0.988939	0.503918	0.0168*
H2c10b	0.59503	1.021837	0.630526	0.0168*
H1c11b	0.285747	1.056606	0.77445	0.0199*
H2c11b	0.273235	1.0641	0.552719	0.0199*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1a	0.0181 (2)	0.0121 (2)	0.0204 (2)	0.0014 (2)	−0.00076 (17)	−0.0019 (2)
Br1b	0.0185 (2)	0.0122 (2)	0.0192 (2)	−0.0015 (2)	−0.00028 (17)	−0.0015 (2)
O1a	0.0109 (16)	0.0154 (17)	0.0216 (18)	0.0020 (13)	0.0010 (14)	−0.0024 (15)
O2a	0.0133 (17)	0.0247 (19)	0.0162 (17)	−0.0031 (14)	0.0002 (14)	0.0033 (15)
O1b	0.0106 (16)	0.0154 (17)	0.0249 (19)	−0.0008 (13)	−0.0014 (14)	−0.0021 (15)
O2b	0.0138 (16)	0.0240 (19)	0.0143 (16)	0.0014 (14)	−0.0011 (13)	−0.0026 (14)
N1a	0.0119 (18)	0.015 (2)	0.0133 (18)	−0.0008 (16)	−0.0012 (14)	0.0011 (15)
N2a	0.0125 (18)	0.0143 (19)	0.0146 (19)	−0.0025 (15)	0.0002 (15)	0.0001 (16)
N1b	0.0149 (19)	0.014 (2)	0.015 (2)	0.0022 (16)	0.0014 (16)	0.0023 (16)
N2b	0.0105 (18)	0.0136 (19)	0.015 (2)	−0.0003 (14)	0.0009 (15)	−0.0015 (16)
C1a	0.011 (2)	0.017 (2)	0.009 (2)	0.0011 (18)	−0.0007 (17)	−0.0011 (18)
C2a	0.011 (2)	0.017 (2)	0.0064 (19)	−0.0010 (18)	−0.0020 (16)	0.0004 (17)
C3a	0.008 (2)	0.013 (2)	0.0116 (19)	−0.0002 (17)	−0.0007 (16)	0.0009 (17)
C4a	0.015 (2)	0.011 (2)	0.011 (2)	0.0018 (17)	−0.0019 (17)	−0.0020 (16)
C5a	0.014 (2)	0.016 (2)	0.010 (2)	−0.0047 (18)	−0.0037 (18)	0.0009 (17)
C6a	0.008 (2)	0.022 (3)	0.011 (2)	−0.0001 (19)	−0.0018 (17)	−0.0017 (18)
C7a	0.009 (2)	0.016 (2)	0.010 (2)	−0.0003 (17)	−0.0003 (16)	0.0014 (18)
C8a	0.013 (2)	0.014 (2)	0.019 (3)	−0.0026 (18)	−0.0001 (18)	0.0023 (18)
C9a	0.016 (2)	0.015 (2)	0.016 (2)	−0.0021 (18)	0.0002 (18)	−0.0004 (18)

C10a	0.012 (2)	0.017 (3)	0.016 (2)	0.0000 (19)	−0.0005 (19)	0.0000 (18)
C11a	0.016 (2)	0.019 (3)	0.016 (2)	0.0004 (19)	−0.0018 (19)	−0.0006 (19)
C1b	0.012 (2)	0.017 (2)	0.010 (2)	−0.0011 (18)	0.0033 (17)	−0.0001 (18)
C2b	0.013 (2)	0.015 (2)	0.008 (2)	0.0004 (18)	0.0011 (17)	0.0010 (18)
C3b	0.009 (2)	0.013 (2)	0.011 (2)	0.0007 (17)	−0.0004 (16)	0.0014 (17)
C4b	0.016 (2)	0.013 (2)	0.010 (2)	−0.0021 (18)	0.0012 (18)	−0.0023 (17)
C5b	0.015 (2)	0.013 (2)	0.011 (2)	0.0054 (18)	0.0016 (18)	0.0005 (17)
C6b	0.009 (2)	0.019 (2)	0.013 (2)	−0.0006 (18)	0.0011 (19)	0.0013 (19)
C7b	0.009 (2)	0.018 (2)	0.013 (2)	0.0005 (18)	0.0008 (17)	0.0010 (18)
C8b	0.018 (3)	0.015 (3)	0.019 (3)	0.0007 (17)	0.004 (2)	−0.0006 (18)
C9b	0.012 (2)	0.013 (2)	0.014 (2)	0.0019 (17)	0.0001 (18)	0.0003 (18)
C10b	0.011 (2)	0.018 (3)	0.013 (2)	0.0013 (18)	0.0028 (19)	0.0015 (17)
C11b	0.016 (2)	0.014 (2)	0.020 (2)	0.0017 (19)	0.001 (2)	0.0009 (19)

Geometric parameters (Å, º)

Br1a—C4a	1.906 (5)	C8a—C9a	1.528 (7)
Br1b—C4b	1.904 (5)	C8a—H1c8a	0.96
O1a—C1a	1.352 (6)	C8a—H2c8a	0.96
O1a—H1o1a	0.82 (5)	C9a—H1c9a	0.96
O2a—C11a	1.425 (6)	C9a—H2c9a	0.96
O2a—H1o2a	0.82 (3)	C10a—C11a	1.520 (7)
O1b—C1b	1.345 (6)	C10a—H1c10a	0.96
O1b—H1o1b	0.82 (5)	C10a—H2c10a	0.96
O2b—C11b	1.429 (6)	C11a—H1c11a	0.96
O2b—H1o2b	0.82 (3)	C11a—H2c11a	0.96
N1a—C7a	1.273 (6)	C1b—C2b	1.411 (7)
N1a—C8a	1.460 (6)	C1b—C6b	1.393 (7)
N2a—C9a	1.460 (6)	C2b—C3b	1.411 (7)
N2a—C10a	1.467 (7)	C2b—C7b	1.460 (7)
N2a—H1n2a	0.88 (3)	C3b—C4b	1.387 (7)
N1b—C7b	1.276 (7)	C3b—H1c3b	0.96
N1b—C8b	1.455 (7)	C4b—C5b	1.382 (7)
N2b—C9b	1.461 (6)	C5b—C6b	1.390 (7)
N2b—C10b	1.472 (7)	C5b—H1c5b	0.96
N2b—H1n2b	0.88 (3)	C6b—H1c6b	0.96
C1a—C2a	1.417 (7)	C7b—H1c7b	0.96
C1a—C6a	1.388 (7)	C8b—C9b	1.530 (7)
C2a—C3a	1.400 (7)	C8b—H1c8b	0.96
C2a—C7a	1.465 (7)	C8b—H2c8b	0.96
C3a—C4a	1.384 (7)	C9b—H1c9b	0.96
C3a—H1c3a	0.96	C9b—H2c9b	0.96
C4a—C5a	1.387 (7)	C10b—C11b	1.519 (7)
C5a—C6a	1.387 (7)	C10b—H1c10b	0.96
C5a—H1c5a	0.96	C10b—H2c10b	0.96
C6a—H1c6a	0.96	C11b—H1c11b	0.96
C7a—H1c7a	0.96	C11b—H2c11b	0.96

C1a—O1a—H1o1a	112 (4)	O2a—C11a—C10a	111.3 (4)
C11a—O2a—H1o2a	101 (5)	O2a—C11a—H1c11a	109.47
C1b—O1b—H1o1b	115 (4)	O2a—C11a—H2c11a	109.47
C11b—O2b—H1o2b	105 (5)	C10a—C11a—H1c11a	109.47
C7a—N1a—C8a	118.0 (4)	C10a—C11a—H2c11a	109.47
C9a—N2a—C10a	111.6 (4)	H1c11a—C11a—H2c11a	107.54
C9a—N2a—H1n2a	113 (4)	O1b—C1b—C2b	121.2 (4)
C10a—N2a—H1n2a	109 (4)	O1b—C1b—C6b	119.1 (4)
C7b—N1b—C8b	117.9 (4)	C2b—C1b—C6b	119.7 (5)
C9b—N2b—C10b	112.2 (4)	C1b—C2b—C3b	119.1 (4)
C9b—N2b—H1n2b	108 (4)	C1b—C2b—C7b	120.6 (4)
C10b—N2b—H1n2b	105 (4)	C3b—C2b—C7b	119.6 (4)
O1a—C1a—C2a	121.3 (4)	C2b—C3b—C4b	119.5 (4)
O1a—C1a—C6a	119.5 (4)	C2b—C3b—H1c3b	120.24
C2a—C1a—C6a	119.2 (4)	C4b—C3b—H1c3b	120.24
C1a—C2a—C3a	119.4 (4)	Br1b—C4b—C3b	118.6 (4)
C1a—C2a—C7a	120.9 (4)	Br1b—C4b—C5b	119.7 (4)
C3a—C2a—C7a	119.4 (4)	C3b—C4b—C5b	121.5 (4)
C2a—C3a—C4a	119.5 (4)	C4b—C5b—C6b	119.4 (4)
C2a—C3a—H1c3a	120.23	C4b—C5b—H1c5b	120.31
C4a—C3a—H1c3a	120.23	C6b—C5b—H1c5b	120.31
Br1a—C4a—C3a	118.9 (4)	C1b—C6b—C5b	120.8 (4)
Br1a—C4a—C5a	119.3 (4)	C1b—C6b—H1c6b	119.6
C3a—C4a—C5a	121.7 (4)	C5b—C6b—H1c6b	119.6
C4a—C5a—C6a	118.8 (4)	N1b—C7b—C2b	121.7 (4)
C4a—C5a—H1c5a	120.6	N1b—C7b—H1c7b	119.13
C6a—C5a—H1c5a	120.6	C2b—C7b—H1c7b	119.13
C1a—C6a—C5a	121.4 (5)	N1b—C8b—C9b	112.0 (4)
C1a—C6a—H1c6a	119.31	N1b—C8b—H1c8b	109.47
C5a—C6a—H1c6a	119.31	N1b—C8b—H2c8b	109.47
N1a—C7a—C2a	121.5 (4)	C9b—C8b—H1c8b	109.47
N1a—C7a—H1c7a	119.24	C9b—C8b—H2c8b	109.47
C2a—C7a—H1c7a	119.24	H1c8b—C8b—H2c8b	106.79
N1a—C8a—C9a	109.3 (4)	N2b—C9b—C8b	109.5 (4)
N1a—C8a—H1c8a	109.47	N2b—C9b—H1c9b	109.47
N1a—C8a—H2c8a	109.47	N2b—C9b—H2c9b	109.47
C9a—C8a—H1c8a	109.47	C8b—C9b—H1c9b	109.47
C9a—C8a—H2c8a	109.47	C8b—C9b—H2c9b	109.47
H1c8a—C8a—H2c8a	109.64	H1c9b—C9b—H2c9b	109.45
N2a—C9a—C8a	111.0 (4)	N2b—C10b—C11b	109.7 (4)
N2a—C9a—H1c9a	109.47	N2b—C10b—H1c10b	109.47
N2a—C9a—H2c9a	109.47	N2b—C10b—H2c10b	109.47
C8a—C9a—H1c9a	109.47	C11b—C10b—H1c10b	109.47
C8a—C9a—H2c9a	109.47	C11b—C10b—H2c10b	109.47
H1c9a—C9a—H2c9a	107.95	H1c10b—C10b—H2c10b	109.22
N2a—C10a—C11a	110.8 (4)	O2b—C11b—C10b	111.6 (4)
N2a—C10a—H1c10a	109.47	O2b—C11b—H1c11b	109.47
N2a—C10a—H2c10a	109.47	O2b—C11b—H2c11b	109.47

C11a—C10a—H1c10a	109.47	C10b—C11b—H1c11b	109.47
C11a—C10a—H2c10a	109.47	C10b—C11b—H2c11b	109.47
H1c10a—C10a—H2c10a	108.1	H1c11b—C11b—H2c11b	107.25

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*a*—H1*o*1*a*···N1*a*	0.82 (5)	1.89 (6)	2.597 (5)	144 (5)
O1*a*—H1*o*1*a*···C7*a*	0.82 (5)	2.45 (6)	2.876 (6)	113 (4)
O2*a*—H1*o*2*a*···N2*b*^{i}	0.82 (3)	2.02 (4)	2.826 (6)	168 (6)
O1*b*—H1*o*1*b*···N1*b*	0.82 (5)	1.91 (6)	2.587 (6)	139 (5)
O2*b*—H1*o*2*b*···N2*a*^{ii}	0.82 (3)	2.06 (4)	2.859 (6)	165 (6)
N2*a*—H1*n*2*a*···O2*a*	0.88 (3)	2.45 (5)	2.871 (6)	110 (5)
N2*b*—H1*n*2*b*···O2*b*	0.88 (3)	2.44 (5)	2.884 (5)	112 (5)

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