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Histamine perchlorate

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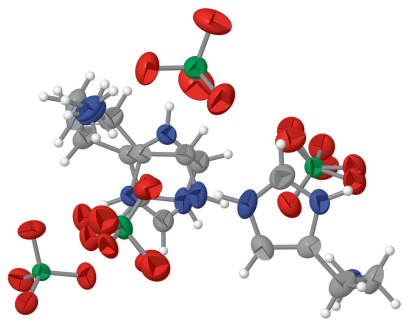
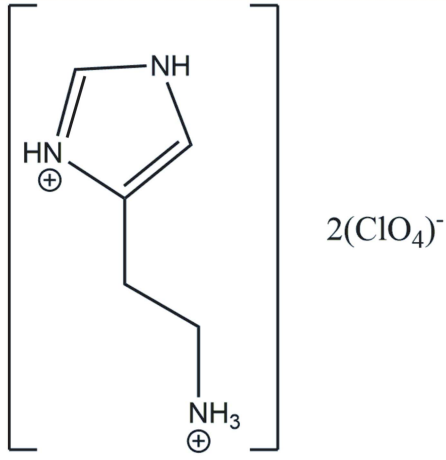
The perchlorate salt of the histamine dication [systematic name: 4-(2-azaniumylethyl)-1*H*-imidazol-3-ium bis(perchlorate)], $C_5H_{11}N_3^{2+}\cdot 2ClO_4^-$, crystallizes in the monoclinic space group $P2_1/c$ with two formula units in the asymmetric unit. One of the histamine dications is disordered [occupancies of 0.718 (4) and 0.282 (4)] and two of the four perchlorate anions are disordered [occupancies of 0.735 (6):0.265 (6) and 0.637 (5):0.363 (5)]. There is extensive hydrogen bonding in the structure involving both N—H···O and C—H···O interactions, which link the histamine dications and perchlorate anions into a three-dimensional array.

3D view



Chemical scheme



Structure description

Histamine is a biologically important compound in the body's immune system (Schneider *et al.*, 2014). It contains an imidazole group which is a nitrogenous aromatic compound found in enzymes and in various drugs (Zlomuzica *et al.*, 2016). Histamines are of interest spanning a wide variety of topics, including drug therapeutics (Zlomuzica *et al.*, 2016), cancer (Martinel Lamas *et al.*, 2015), addictions (Nuutinen *et al.*, 2016), and autoimmune (Abiuso *et al.*, 2014) and anxiety disorders (Cacabelos *et al.*, 2016). In view of this interest in histamine, several structures of histamine salts have been determined through X-ray crystallography previously containing both histamine dications (Veidis *et al.*, 1969; Yamane *et al.*, 1973) and histamine cations (Prout *et al.*, 1974; Belfilali *et al.*, 2015).

The present report contains the structure of the perchlorate salt of histamine in the diprotonated form, which crystallizes in the monoclinic space group $P2_1/c$ with two formula units in the asymmetric unit (Fig. 1). One of the histamine dications is disordered [occupancies of 0.718 (4) and 0.282 (4)] and two of the four perchlorate anions are disordered [occupancies of 0.735 (6):0.265 (6) and 0.637 (5):0.363 (5)]. The metrical parameters of the diprotonated imidazolium ring are similar to those found for the

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

D—H···A	D—H	H···A	D···A	D—H···A
N1A—H1A···O13^{i}	0.88	2.50	3.337 (4)	160
N1A—H1A···O14^{i}	0.88	2.49	3.052 (4)	122
N1A—H1A···O43^{ii}	0.88	2.47	3.021 (7)	121
N1A—H1A···O41A^{ii}	0.88	2.36	2.978 (9)	127
N2A—H2A···Cl4	0.88	2.96	3.709 (3)	145
N2A—H2A···O41	0.88	2.03	2.907 (9)	171
N2A—H2A···O44A	0.88	2.08	2.95 (2)	168
N3A—H3A1···O21^{iii}	0.91	2.56	3.040 (4)	114
N3A—H3A1···O34^{iv}	0.91	2.23	3.065 (6)	153
N3A—H3A1···O33A^{iv}	0.91	2.11	2.861 (12)	139
N3A—H3A2···Cl1^{v}	0.91	2.98	3.742 (3)	143
N3A—H3A2···O11^{v}	0.91	2.45	3.031 (4)	122
N3A—H3A2···O12^{v}	0.91	2.44	3.232 (4)	146
N3A—H3A2···O42^{v}	0.91	2.53	3.207 (8)	131
N3A—H3A2···O42A^{v}	0.91	2.57	3.272 (14)	134
N3A—H3A3···Cl3	0.91	2.95	3.735 (3)	145
N3A—H3A3···O31	0.91	2.51	3.055 (8)	119
N3A—H3A3···O32	0.91	2.26	3.120 (8)	159
N3A—H3A3···O32A	0.91	2.14	3.04 (2)	170
C2A—H2AA···O14^{i}	0.95	2.65	3.129 (5)	112
C2A—H2AA···O22	0.95	2.40	3.074 (5)	128
C4A—H4AB···O43^{ii}	0.99	2.66	3.379 (8)	129
C5A—H5AA···O42^{v}	0.99	2.70	3.158 (9)	109
C5A—H5AA···O43^{v}	0.99	2.70	3.310 (7)	120
C5A—H5AB···O12^{vi}	0.99	2.61	3.542 (5)	158
N1B—H1B···Cl1	0.88	2.91	3.714 (5)	153
N1B—H1B···O12	0.88	2.39	3.265 (6)	171
N1B—H1B···O14	0.88	2.38	2.961 (6)	124
N2B—H2B···O32	0.88	2.10	2.939 (9)	159
N3B—H3B1···Cl4	0.91	2.94	3.695 (14)	142
N3B—H3B1···O41	0.91	2.05	2.937 (19)	163
N3B—H3B1···O42	0.91	2.65	3.168 (13)	117
N3B—H3B2···O11^{vii}	0.91	2.56	3.120 (14)	120
N3B—H3B2···O13^{vii}	0.91	2.45	3.269 (11)	150
N3B—H3B2···O31^{viii}	0.91	2.63	3.310 (14)	132
N3B—H3B3···O21	0.91	2.36	2.910 (10)	119
N3B—H3B3···O34^{ix}	0.91	2.56	3.374 (13)	150
C1B—H1BA···O24^{ix}	0.95	2.64	3.441 (7)	142
C2B—H2BA···O22^{iii}	0.95	2.50	3.024 (6)	115
C4B—H4BB···O33^{ix}	0.99	2.50	3.433 (8)	156
C5B—H5BA···O11^{x}	0.99	2.52	3.249 (10)	130
N2BA—H2B1···O22^{iii}	0.88	2.38	3.150 (15)	146
N3BA—H3B4···Cl1^{vii}	0.91	2.78	3.62 (3)	155
N3BA—H3B4···O11^{vii}	0.91	2.15	2.93 (4)	144
N3BA—H3B4···O13^{vii}	0.91	2.40	3.12 (3)	137
N3BA—H3B4···O31A^{viii}	0.91	2.59	3.14 (4)	120
N3BA—H3B5···Cl2	0.91	2.82	3.66 (3)	154
N3BA—H3B5···O21	0.91	2.13	2.83 (2)	133
N3BA—H3B5···O24	0.91	2.48	3.29 (4)	149
N3BA—H3B6···Cl4	0.91	2.87	3.77 (4)	168
N3BA—H3B6···O44A	0.91	2.28	3.07 (5)	146
C1BA—H1BB···O14	0.95	2.16	3.103 (17)	171
C2BA—H2BB···Cl3	0.95	2.75	3.644 (14)	157
C2BA—H2BB···O32A	0.95	2.46	3.12 (3)	127
C2BA—H2BB···O34A	0.95	2.09	3.04 (2)	173
C4BA—H4BD···O11^{x}	0.99	2.56	3.250 (13)	127
C4BA—H4BC···O12	0.99	2.38	3.325 (16)	159
C5BA—H5BC···Cl3^{ix}	0.99	2.98	3.86 (3)	149
C5BA—H5BC···O34A^{ix}	0.99	2.26	3.18 (4)	153
C5BA—H5BD···O31A^{viii}	0.99	2.57	3.22 (4)	123

Symmetry codes: (i) $-x+1, y-\frac{1}{2}, -z+\frac{1}{2}$; (ii) $-x+1, -y+1, -z+1$; (iii) $-x+1, y+\frac{1}{2}, -z+\frac{1}{2}$; (iv) $x, -y+\frac{3}{2}, z+\frac{1}{2}$; (v) $x-1, y, z$; (vi) $x-1, -y+\frac{3}{2}, z+\frac{1}{2}$; (vii) $-x+2, y-\frac{1}{2}, -z+\frac{1}{2}$; (viii) $x+1, y, z$; (ix) $-x+1, -y+1, -z$; (x) $x, -y+\frac{3}{2}, z-\frac{1}{2}$.

phosphate (Veidis *et al.*, 1969) and sulfate analogs (Yamane *et al.*, 1973). It has been suggested (Kier, 1968) that the dual activity of histamine is a consequence of the ability of its monocation to adopt two distinct preferred conformations,

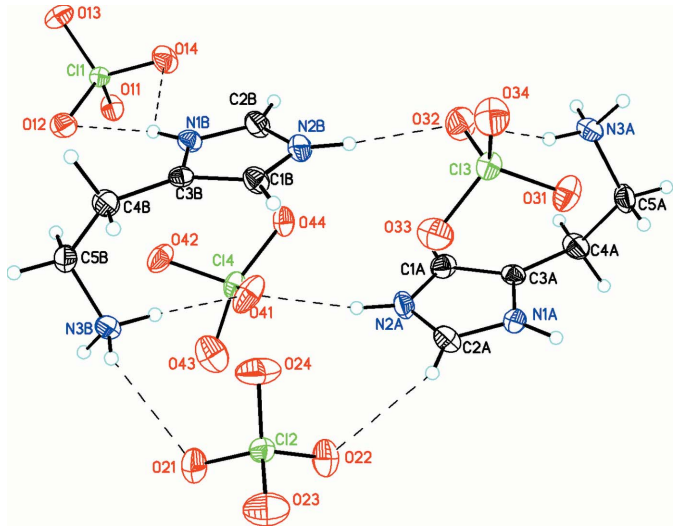


Figure 1
Diagram showing the histamine dication and perchlorate anions (major component only for disordered species) and the atom labeling. Atomic displacement parameters are at the 50% probability level. N—H···O and C—H···O hydrogen-bond interactions are indicated by dashed bonds.

viz. *trans* and *gauche* rotamers involving the ethanamine substituent. In the title compound, there are two independent histamine dications and one of them is disordered over two conformations. The three C3—C4—C5—N3 torsion angles are −64.3 (5), 59.4 (7), and −50 (2)°. These values are in contrast to the values reported in the two structures containing histamine cations where these torsion angles are 177.3 (Prout *et al.*, 1974) and 176.22 (10)° (Belfilali *et al.*, 2015).

There is extensive hydrogen bonding in the structure, involving both N—H···O and C—H···O interactions, which link the histamine dications and perchlorate anions into a three-dimensional array (Table 1 and Fig. 2).

Synthesis and crystallization

Histamine hydrochloride (0.3181 g, 1.728 mmol) was dissolved in 15 ml of methanol. $Zn(ClO_4)_2{\cdot}6H_2O$ (0.6434 g, 1.728 mmol) was dissolved in 15 ml of methanol and added to the histamine hydrochloride solution. The mixture was stirred at room

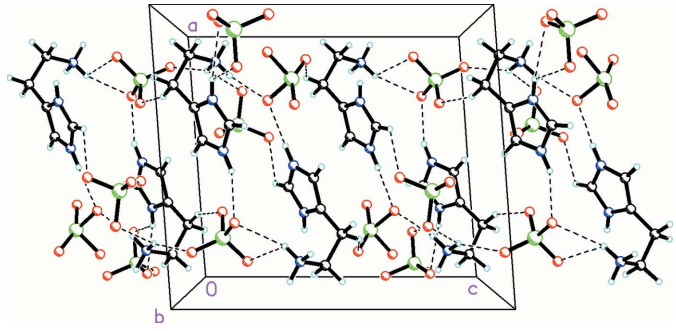


Figure 2
Packing diagram for the title compound, viewed along the *b* axis, showing the three-dimensional arrangement. N—H···O and C—H···O hydrogen-bond interactions are indicated by dashed bonds.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_5H_{11}N_3^{2+}\cdot 2ClO_4^-$
M_r	312.07
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	173
a, b, c (Å)	11.3333 (6), 16.4178 (9), 12.7650 (6)
β (°)	94.140 (5)
V (Å^3)	2369.0 (2)
Z	8
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.59
Crystal size (mm)	0.43 × 0.37 × 0.27
Data collection	
Diffractometer	Oxford Diffraction Xcalibur Eos Gemini
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku-Oxford Diffraction, 2015)
T_{min}, T_{max}	0.765, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	12472, 5581, 3463
R_{int}	0.034
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.686
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.063, 0.219, 1.07
No. of reflections	5581
No. of parameters	380
No. of restraints	450
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.91, −0.63

Computer programs: *CrysAlis PRO* (Rigaku-Oxford Diffraction, 2015), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*) and *SHELXTL* (Sheldrick, 2008).

temperature overnight. The methanol was removed by rotary evaporation. The product was crystallized by redissolving it in acetonitrile and layering the solution with diethyl ether. After ∼1 h, a colorless crystal formed. The crystal was allowed to grow overnight before gravity filtration, air drying, and collection of the crystallized product for XRD analysis.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. One of the histamine dications is disordered [occupancies of 0.718 (4) and 0.282 (4)] and both components were constrained to have similar metrical parameters. Two of the four perchlorate anions are also disordered [occupancies of 0.735 (6):0.265 (6) and 0.637 (5):0.363 (5)] and were constrained to be tetrahedral.

All of the H atoms were placed in calculated positions and then refined using the riding model, with C/N—H = 0.95 (CH), 0.88 (NH), 0.99 (CH_2), or 0.91 Å (NH_3). Isotropic displacement parameters for these atoms were set at 1.2 (CH, NH and CH_2) or 1.5 (NH_3) times U_{eq} of the parent atom. The H atoms for the idealized ammonium groups were refined as rotating groups.

Acknowledgements

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full crystallographic data

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4-(2-Azaniumylethyl)-1*H*-imidazol-3-ium bis(perchlorate)

Crystal data

$C_5H_{11}N_3^{2+}\cdot 2ClO_4^-$
M_r = 312.07
Monoclinic, $P2_1/c$
a = 11.3333 (6) Å
b = 16.4178 (9) Å
c = 12.7650 (6) Å
β = 94.140 (5)°
V = 2369.0 (2) Å^3
Z = 8
F(000) = 1280
D_x = 1.750 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2709 reflections
θ = 4.0–27.7°
μ = 0.59 mm^{-1}
T = 173 K
Chunk, colorless
0.43 × 0.37 × 0.27 mm

Data collection

Oxford Diffraction Xcalibur Eos Gemini diffractometer
Radiation source: fine-focus sealed X-ray tube
Detector resolution: 16.0416 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlis PRO; Rigaku-Oxford Diffraction, 2015)
T_{min} = 0.765, T_{max} = 1.000
12472 measured reflections
5581 independent reflections
3463 reflections with $I > 2\sigma(I)$
R_{int} = 0.034
θ_{max} = 29.2°, θ_{min} = 3.4°
$h = -15\rightarrow 14$
$k = -21\rightarrow 19$
$l = -17\rightarrow 14$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.063
$wR(F^2)$ = 0.219
S = 1.07
5581 reflections
380 parameters
450 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1133P)^2 + 0.5966P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.91 e Å^{-3}
$\Delta\rho_{min}$ = −0.63 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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Cl1	0.93140 (7)	0.87376 (4)	0.23249 (6)	0.0358 (2)	
O11	0.9819 (2)	0.87540 (14)	0.3395 (2)	0.0543 (7)	
O12	0.9664 (3)	0.79992 (15)	0.1841 (2)	0.0615 (8)	
O13	0.9715 (3)	0.94274 (15)	0.1778 (2)	0.0636 (8)	
O14	0.8045 (2)	0.87571 (15)	0.2327 (3)	0.0640 (8)	
Cl2	0.62291 (9)	0.37350 (5)	0.18816 (8)	0.0497 (3)	
O21	0.7507 (3)	0.37336 (18)	0.2093 (3)	0.0798 (10)	
O22	0.5747 (3)	0.37663 (18)	0.2888 (3)	0.0847 (11)	
O23	0.5902 (4)	0.30024 (19)	0.1372 (3)	0.0986 (13)	
O24	0.5900 (4)	0.44327 (19)	0.1284 (3)	0.0987 (13)	
Cl3	0.20743 (8)	0.61832 (5)	0.13100 (7)	0.0455 (3)	
O31	0.1200 (7)	0.5955 (5)	0.2027 (6)	0.0676 (17)	0.735 (12)
O32	0.2645 (6)	0.6896 (4)	0.1755 (6)	0.0710 (17)	0.735 (12)
O33	0.2975 (5)	0.5553 (3)	0.1305 (6)	0.0752 (14)	0.735 (12)
O34	0.1566 (5)	0.6322 (5)	0.0292 (4)	0.0736 (15)	0.735 (12)
O31A	0.1243 (19)	0.5737 (13)	0.1863 (17)	0.0676 (17)	0.265 (12)
O32A	0.2797 (19)	0.6680 (11)	0.2011 (15)	0.0710 (17)	0.265 (12)
O33A	0.1424 (13)	0.6683 (10)	0.0529 (12)	0.0752 (14)	0.265 (12)
O34A	0.2837 (12)	0.5632 (9)	0.0836 (13)	0.0736 (15)	0.265 (12)
Cl4	0.78058 (8)	0.62532 (5)	0.38789 (7)	0.0487 (3)	
O41	0.7113 (8)	0.5720 (6)	0.3164 (5)	0.0618 (12)	0.637 (8)
O42	0.8672 (6)	0.6601 (4)	0.3188 (6)	0.0583 (16)	0.637 (8)
O43	0.8519 (5)	0.5664 (4)	0.4510 (5)	0.0800 (14)	0.637 (8)
O44	0.6998 (6)	0.6864 (4)	0.4113 (7)	0.100 (2)	0.637 (8)
O41A	0.8376 (8)	0.6002 (7)	0.4848 (6)	0.0618 (12)	0.363 (8)
O42A	0.8479 (12)	0.6845 (7)	0.3473 (10)	0.0583 (16)	0.363 (8)
O43A	0.6992 (9)	0.6577 (7)	0.4652 (8)	0.0800 (14)	0.363 (8)
O44A	0.7187 (17)	0.5708 (12)	0.3267 (14)	0.100 (2)	0.363 (8)
N1A	0.2935 (3)	0.52105 (17)	0.3947 (3)	0.0501 (8)	
H1A	0.2274	0.4928	0.3904	0.060*	
N2A	0.4681 (3)	0.5565 (2)	0.3720 (3)	0.0569 (8)	
H2A	0.5400	0.5570	0.3502	0.068*	
N3A	0.1315 (3)	0.72364 (18)	0.3767 (2)	0.0496 (8)	
H3A1	0.1619	0.7684	0.4110	0.074*	
H3A2	0.0614	0.7368	0.3414	0.074*	
H3A3	0.1831	0.7059	0.3303	0.074*	
C1A	0.4234 (4)	0.6133 (2)	0.4349 (3)	0.0531 (10)	
H1AA	0.4638	0.6599	0.4632	0.064*	
C2A	0.3886 (4)	0.5012 (3)	0.3488 (3)	0.0609 (11)	
H2AA	0.3981	0.4547	0.3060	0.073*	
C3A	0.3104 (3)	0.5915 (2)	0.4503 (3)	0.0430 (8)	
C4A	0.2219 (4)	0.6305 (3)	0.5131 (3)	0.0616 (11)	
H4AA	0.2593	0.6780	0.5498	0.074*	
H4AB	0.1999	0.5914	0.5674	0.074*	
C5A	0.1121 (4)	0.6584 (3)	0.4536 (3)	0.0612 (11)	

H5AA	0.0746	0.6113	0.4160	0.073*	
H5AB	0.0563	0.6784	0.5040	0.073*	
N1B	0.7010 (4)	0.7247 (4)	0.1384 (6)	0.0428 (10)	0.718 (4)
H1B	0.7702	0.7491	0.1450	0.051*	0.718 (4)
N2B	0.5215 (5)	0.6944 (3)	0.1579 (6)	0.0585 (13)	0.718 (4)
H2B	0.4501	0.6953	0.1806	0.070*	0.718 (4)
N3B	0.8500 (14)	0.5260 (5)	0.1399 (9)	0.0632 (17)	0.718 (4)
H3B1	0.7964	0.5442	0.1842	0.095*	0.718 (4)
H3B2	0.9194	0.5145	0.1773	0.095*	0.718 (4)
H3B3	0.8219	0.4801	0.1069	0.095*	0.718 (4)
C1B	0.5590 (5)	0.6422 (4)	0.0889 (6)	0.0502 (14)	0.718 (4)
H1BA	0.5131	0.6001	0.0551	0.060*	0.718 (4)
C2B	0.6104 (5)	0.7464 (3)	0.1882 (5)	0.0560 (14)	0.718 (4)
H2BA	0.6069	0.7902	0.2365	0.067*	0.718 (4)
C3B	0.6760 (4)	0.6593 (4)	0.0743 (6)	0.0369 (11)	0.718 (4)
C4B	0.7598 (6)	0.6220 (3)	0.0064 (4)	0.0544 (13)	0.718 (4)
H4BA	0.7827	0.6633	−0.0449	0.065*	0.718 (4)
H4BB	0.7190	0.5773	−0.0337	0.065*	0.718 (4)
C5B	0.8697 (9)	0.5887 (5)	0.0620 (8)	0.0580 (19)	0.718 (4)
H5BA	0.9200	0.5655	0.0091	0.070*	0.718 (4)
H5BB	0.9141	0.6341	0.0973	0.070*	0.718 (4)
N1BA	0.6110 (10)	0.6215 (6)	0.0500 (9)	0.0428 (10)	0.282 (4)
H1B1	0.6061	0.5802	0.0060	0.051*	0.282 (4)
N2BA	0.5560 (13)	0.7150 (10)	0.1540 (16)	0.0585 (13)	0.282 (4)
H2B1	0.5131	0.7459	0.1929	0.070*	0.282 (4)
N3BA	0.861 (4)	0.5172 (14)	0.142 (2)	0.0632 (17)	0.282 (4)
H3B4	0.9298	0.4911	0.1616	0.095*	0.282 (4)
H3B5	0.8023	0.4799	0.1290	0.095*	0.282 (4)
H3B6	0.8414	0.5506	0.1954	0.095*	0.282 (4)
C1BA	0.6727 (14)	0.7246 (14)	0.137 (2)	0.0502 (14)	0.282 (4)
H1BB	0.7209	0.7680	0.1642	0.060*	0.282 (4)
C2BA	0.5214 (13)	0.6495 (11)	0.1002 (17)	0.0560 (14)	0.282 (4)
H2BB	0.4445	0.6262	0.0979	0.067*	0.282 (4)
C3BA	0.7112 (11)	0.6643 (12)	0.0744 (18)	0.0369 (11)	0.282 (4)
C4BA	0.8326 (12)	0.6508 (8)	0.0449 (12)	0.0544 (13)	0.282 (4)
H4BC	0.8868	0.6838	0.0922	0.065*	0.282 (4)
H4BD	0.8384	0.6718	−0.0273	0.065*	0.282 (4)
C5BA	0.875 (3)	0.5654 (13)	0.048 (2)	0.0580 (19)	0.282 (4)
H5BC	0.8344	0.5362	−0.0118	0.070*	0.282 (4)
H5BD	0.9605	0.5662	0.0363	0.070*	0.282 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0371 (4)	0.0371 (4)	0.0329 (4)	−0.0003 (3)	−0.0002 (3)	−0.0012 (3)
O11	0.0487 (16)	0.0773 (19)	0.0359 (14)	0.0074 (12)	−0.0038 (12)	−0.0022 (11)
O12	0.086 (2)	0.0446 (14)	0.0553 (16)	0.0066 (13)	0.0168 (15)	−0.0084 (12)
O13	0.086 (2)	0.0480 (15)	0.0568 (17)	−0.0153 (14)	0.0066 (15)	0.0095 (12)

O14	0.0365 (15)	0.074 (2)	0.080 (2)	0.0016 (12)	−0.0089 (14)	0.0016 (14)
Cl2	0.0541 (6)	0.0417 (5)	0.0543 (6)	−0.0012 (4)	0.0103 (5)	−0.0003 (4)
O21	0.0537 (19)	0.093 (3)	0.095 (3)	−0.0011 (14)	0.0224 (18)	0.0046 (17)
O22	0.074 (2)	0.106 (3)	0.078 (2)	0.0017 (16)	0.0317 (19)	−0.0042 (17)
O23	0.131 (3)	0.0587 (18)	0.104 (3)	−0.0135 (19)	−0.012 (2)	−0.0211 (18)
O24	0.118 (3)	0.0599 (19)	0.114 (3)	0.0027 (19)	−0.022 (2)	0.0284 (19)
Cl3	0.0448 (5)	0.0536 (5)	0.0378 (5)	−0.0062 (4)	0.0013 (4)	−0.0008 (4)
O31	0.064 (2)	0.089 (4)	0.051 (3)	−0.021 (3)	0.0095 (18)	0.003 (3)
O32	0.061 (3)	0.067 (3)	0.085 (4)	−0.013 (3)	0.002 (2)	−0.012 (3)
O33	0.092 (3)	0.075 (2)	0.058 (3)	0.018 (2)	0.005 (2)	0.002 (2)
O34	0.075 (3)	0.103 (4)	0.043 (2)	0.002 (2)	−0.0017 (19)	0.005 (2)
O31A	0.064 (2)	0.089 (4)	0.051 (3)	−0.021 (3)	0.0095 (18)	0.003 (3)
O32A	0.061 (3)	0.067 (3)	0.085 (4)	−0.013 (3)	0.002 (2)	−0.012 (3)
O33A	0.092 (3)	0.075 (2)	0.058 (3)	0.018 (2)	0.005 (2)	0.002 (2)
O34A	0.075 (3)	0.103 (4)	0.043 (2)	0.002 (2)	−0.0017 (19)	0.005 (2)
Cl4	0.0430 (5)	0.0639 (6)	0.0390 (5)	−0.0147 (4)	0.0025 (4)	−0.0020 (4)
O41	0.050 (2)	0.093 (3)	0.042 (2)	−0.033 (2)	0.0045 (18)	−0.017 (2)
O42	0.048 (3)	0.073 (4)	0.054 (4)	−0.015 (3)	0.005 (2)	0.011 (3)
O43	0.084 (3)	0.093 (3)	0.062 (3)	−0.012 (2)	0.001 (2)	−0.002 (2)
O44	0.088 (3)	0.104 (4)	0.112 (5)	−0.017 (3)	0.040 (3)	−0.057 (4)
O41A	0.050 (2)	0.093 (3)	0.042 (2)	−0.033 (2)	0.0045 (18)	−0.017 (2)
O42A	0.048 (3)	0.073 (4)	0.054 (4)	−0.015 (3)	0.005 (2)	0.011 (3)
O43A	0.084 (3)	0.093 (3)	0.062 (3)	−0.012 (2)	0.001 (2)	−0.002 (2)
O44A	0.088 (3)	0.104 (4)	0.112 (5)	−0.017 (3)	0.040 (3)	−0.057 (4)
N1A	0.0401 (16)	0.0467 (16)	0.064 (2)	−0.0047 (12)	0.0047 (14)	0.0039 (14)
N2A	0.0340 (16)	0.076 (2)	0.062 (2)	0.0107 (15)	0.0091 (15)	0.0117 (17)
N3A	0.0545 (19)	0.0522 (17)	0.0420 (16)	0.0164 (14)	0.0032 (14)	0.0018 (14)
C1A	0.049 (2)	0.049 (2)	0.059 (2)	−0.0084 (16)	−0.0074 (18)	0.0042 (17)
C2A	0.055 (2)	0.058 (2)	0.070 (3)	0.0147 (18)	0.006 (2)	−0.002 (2)
C3A	0.051 (2)	0.0427 (18)	0.0352 (17)	0.0103 (15)	0.0029 (15)	0.0094 (15)
C4A	0.065 (3)	0.075 (3)	0.045 (2)	0.021 (2)	0.0090 (19)	0.0111 (18)
C5A	0.042 (2)	0.083 (3)	0.061 (2)	0.013 (2)	0.0187 (18)	0.014 (2)
N1B	0.040 (2)	0.0394 (19)	0.049 (2)	0.0023 (19)	−0.003 (2)	0.0004 (16)
N2B	0.036 (3)	0.059 (3)	0.080 (3)	0.0010 (19)	0.005 (2)	0.008 (3)
N3B	0.074 (4)	0.052 (3)	0.067 (2)	0.024 (3)	0.028 (2)	0.012 (2)
C1B	0.041 (3)	0.051 (3)	0.058 (3)	0.003 (2)	−0.002 (2)	−0.006 (2)
C2B	0.043 (3)	0.052 (3)	0.072 (3)	0.005 (2)	0.002 (2)	−0.006 (2)
C3B	0.040 (3)	0.0350 (19)	0.0348 (18)	0.002 (2)	−0.005 (3)	0.0048 (15)
C4B	0.060 (3)	0.061 (3)	0.042 (3)	0.013 (2)	0.008 (2)	0.005 (2)
C5B	0.045 (2)	0.068 (5)	0.062 (4)	0.010 (3)	0.017 (2)	0.015 (4)
N1BA	0.040 (2)	0.0394 (19)	0.049 (2)	0.0023 (19)	−0.003 (2)	0.0004 (16)
N2BA	0.036 (3)	0.059 (3)	0.080 (3)	0.0010 (19)	0.005 (2)	0.008 (3)
N3BA	0.074 (4)	0.052 (3)	0.067 (2)	0.024 (3)	0.028 (2)	0.012 (2)
C1BA	0.041 (3)	0.051 (3)	0.058 (3)	0.003 (2)	−0.002 (2)	−0.006 (2)
C2BA	0.043 (3)	0.052 (3)	0.072 (3)	0.005 (2)	0.002 (2)	−0.006 (2)
C3BA	0.040 (3)	0.0350 (19)	0.0348 (18)	0.002 (2)	−0.005 (3)	0.0048 (15)
C4BA	0.060 (3)	0.061 (3)	0.042 (3)	0.013 (2)	0.008 (2)	0.005 (2)
C5BA	0.045 (2)	0.068 (5)	0.062 (4)	0.010 (3)	0.017 (2)	0.015 (4)

Geometric parameters (Å, º)

Cl1—O13	1.422 (3)	C5A—H5AA	0.9900
Cl1—O12	1.430 (2)	C5A—H5AB	0.9900
Cl1—O14	1.439 (3)	N1B—C2B	1.297 (7)
Cl1—O11	1.442 (3)	N1B—C3B	1.367 (7)
Cl2—O23	1.404 (3)	N1B—H1B	0.8800
Cl2—O24	1.412 (3)	N2B—C1B	1.320 (8)
Cl2—O22	1.433 (4)	N2B—C2B	1.355 (7)
Cl2—O21	1.454 (4)	N2B—H2B	0.8800
Cl3—O34	1.402 (4)	N3B—C5B	1.460 (7)
Cl3—O34A	1.417 (11)	N3B—H3B1	0.9100
Cl3—O31A	1.421 (12)	N3B—H3B2	0.9100
Cl3—O32A	1.425 (12)	N3B—H3B3	0.9100
Cl3—O32	1.434 (5)	C1B—C3B	1.381 (8)
Cl3—O31	1.446 (5)	C1B—H1BA	0.9500
Cl3—O33A	1.451 (11)	C2B—H2BA	0.9500
Cl3—O33	1.454 (5)	C3B—C4B	1.465 (7)
Cl4—O44A	1.350 (11)	C4B—C5B	1.493 (10)
Cl4—O42A	1.361 (10)	C4B—H4BA	0.9900
Cl4—O44	1.405 (6)	C4B—H4BB	0.9900
Cl4—O41A	1.415 (8)	C5B—H5BA	0.9900
Cl4—O41	1.454 (5)	C5B—H5BB	0.9900
Cl4—O43	1.465 (5)	N1BA—C2BA	1.322 (13)
Cl4—O42	1.481 (5)	N1BA—C3BA	1.352 (13)
Cl4—O43A	1.496 (9)	N1BA—H1B1	0.8800
N1A—C2A	1.305 (5)	N2BA—C2BA	1.321 (16)
N1A—C3A	1.363 (4)	N2BA—C1BA	1.366 (15)
N1A—H1A	0.8800	N2BA—H2B1	0.8800
N2A—C2A	1.298 (5)	N3BA—C5BA	1.457 (15)
N2A—C1A	1.351 (5)	N3BA—H3B4	0.9100
N2A—H2A	0.8800	N3BA—H3B5	0.9100
N3A—C5A	1.481 (5)	N3BA—H3B6	0.9100
N3A—H3A1	0.9100	C1BA—C3BA	1.360 (15)
N3A—H3A2	0.9100	C1BA—H1BB	0.9500
N3A—H3A3	0.9100	C2BA—H2BB	0.9500
C1A—C3A	1.357 (5)	C3BA—C4BA	1.470 (13)
C1A—H1AA	0.9500	C4BA—C5BA	1.483 (15)
C2A—H2AA	0.9500	C4BA—H4BC	0.9900
C3A—C4A	1.475 (5)	C4BA—H4BD	0.9900
C4A—C5A	1.482 (6)	C5BA—H5BC	0.9900
C4A—H4AA	0.9900	C5BA—H5BD	0.9900
C4A—H4AB	0.9900		
O13—Cl1—O12	110.77 (19)	H5AA—C5A—H5AB	107.7
O13—Cl1—O14	109.79 (18)	C2B—N1B—C3B	111.8 (5)
O12—Cl1—O14	109.18 (17)	C2B—N1B—H1B	124.1
O13—Cl1—O11	109.30 (16)	C3B—N1B—H1B	124.1

O12—Cl1—O11	108.74 (16)	C1B—N2B—C2B	109.3 (5)
O14—Cl1—O11	109.04 (19)	C1B—N2B—H2B	125.3
O23—Cl2—O24	113.2 (3)	C2B—N2B—H2B	125.3
O23—Cl2—O22	109.9 (2)	C5B—N3B—H3B1	109.5
O24—Cl2—O22	110.6 (2)	C5B—N3B—H3B2	109.5
O23—Cl2—O21	108.1 (2)	H3B1—N3B—H3B2	109.5
O24—Cl2—O21	108.8 (2)	C5B—N3B—H3B3	109.5
O22—Cl2—O21	105.9 (2)	H3B1—N3B—H3B3	109.5
O34A—Cl3—O31A	109.3 (10)	H3B2—N3B—H3B3	109.5
O34A—Cl3—O32A	107.0 (10)	N2B—C1B—C3B	108.5 (6)
O31A—Cl3—O32A	110.8 (11)	N2B—C1B—H1BA	125.8
O34—Cl3—O32	112.2 (3)	C3B—C1B—H1BA	125.8
O34—Cl3—O31	112.0 (4)	N1B—C2B—N2B	106.6 (5)
O32—Cl3—O31	105.7 (4)	N1B—C2B—H2BA	126.7
O34A—Cl3—O33A	111.3 (7)	N2B—C2B—H2BA	126.7
O31A—Cl3—O33A	108.1 (11)	N1B—C3B—C1B	103.7 (5)
O32A—Cl3—O33A	110.4 (9)	N1B—C3B—C4B	124.5 (5)
O34—Cl3—O33	110.7 (3)	C1B—C3B—C4B	131.7 (6)
O32—Cl3—O33	106.6 (3)	C3B—C4B—C5B	115.3 (6)
O31—Cl3—O33	109.3 (4)	C3B—C4B—H4BA	108.5
O44A—Cl4—O42A	122.3 (10)	C5B—C4B—H4BA	108.5
O44A—Cl4—O41A	119.9 (10)	C3B—C4B—H4BB	108.5
O42A—Cl4—O41A	107.9 (7)	C5B—C4B—H4BB	108.5
O44—Cl4—O41	103.5 (5)	H4BA—C4B—H4BB	107.5
O44—Cl4—O43	134.2 (6)	N3B—C5B—C4B	114.8 (9)
O41—Cl4—O43	101.5 (5)	N3B—C5B—H5BA	108.6
O44—Cl4—O42	108.7 (4)	C4B—C5B—H5BA	108.6
O41—Cl4—O42	102.1 (4)	N3B—C5B—H5BB	108.6
O43—Cl4—O42	102.7 (4)	C4B—C5B—H5BB	108.6
O44A—Cl4—O43A	107.3 (9)	H5BA—C5B—H5BB	107.6
O42A—Cl4—O43A	112.8 (6)	C2BA—N1BA—C3BA	111.7 (11)
O41A—Cl4—O43A	78.0 (6)	C2BA—N1BA—H1B1	124.1
C2A—N1A—C3A	110.8 (3)	C3BA—N1BA—H1B1	124.1
C2A—N1A—H1A	124.6	C2BA—N2BA—C1BA	105.3 (12)
C3A—N1A—H1A	124.6	C2BA—N2BA—H2B1	127.3
C2A—N2A—C1A	109.5 (3)	C1BA—N2BA—H2B1	127.3
C2A—N2A—H2A	125.2	C5BA—N3BA—H3B4	109.5
C1A—N2A—H2A	125.2	C5BA—N3BA—H3B5	109.5
C5A—N3A—H3A1	109.5	H3B4—N3BA—H3B5	109.5
C5A—N3A—H3A2	109.5	C5BA—N3BA—H3B6	109.5
H3A1—N3A—H3A2	109.5	H3B4—N3BA—H3B6	109.5
C5A—N3A—H3A3	109.5	H3B5—N3BA—H3B6	109.5
H3A1—N3A—H3A3	109.5	C3BA—C1BA—N2BA	111.5 (13)
H3A2—N3A—H3A3	109.5	C3BA—C1BA—H1BB	124.3
N2A—C1A—C3A	107.6 (3)	N2BA—C1BA—H1BB	124.3
N2A—C1A—H1AA	126.2	N2BA—C2BA—N1BA	109.0 (12)
C3A—C1A—H1AA	126.2	N2BA—C2BA—H2BB	125.5
N2A—C2A—N1A	107.8 (4)	N1BA—C2BA—H2BB	125.5

N2A—C2A—H2AA	126.1	N1BA—C3BA—C1BA	102.3 (11)
N1A—C2A—H2AA	126.1	N1BA—C3BA—C4BA	130.5 (14)
C1A—C3A—N1A	104.3 (3)	C1BA—C3BA—C4BA	127.2 (14)
C1A—C3A—C4A	130.6 (4)	C3BA—C4BA—C5BA	116.3 (15)
N1A—C3A—C4A	125.1 (4)	C3BA—C4BA—H4BC	108.2
C3A—C4A—C5A	115.8 (4)	C5BA—C4BA—H4BC	108.2
C3A—C4A—H4AA	108.3	C3BA—C4BA—H4BD	108.2
C5A—C4A—H4AA	108.3	C5BA—C4BA—H4BD	108.2
C3A—C4A—H4AB	108.3	H4BC—C4BA—H4BD	107.4
C5A—C4A—H4AB	108.3	N3BA—C5BA—C4BA	119 (2)
H4AA—C4A—H4AB	107.4	N3BA—C5BA—H5BC	107.6
N3A—C5A—C4A	113.8 (3)	C4BA—C5BA—H5BC	107.6
N3A—C5A—H5AA	108.8	N3BA—C5BA—H5BD	107.6
C4A—C5A—H5AA	108.8	C4BA—C5BA—H5BD	107.6
N3A—C5A—H5AB	108.8	H5BC—C5BA—H5BD	107.0
C4A—C5A—H5AB	108.8		

C2A—N2A—C1A—C3A	−0.3 (5)	N2B—C1B—C3B—N1B	−0.6 (10)
C1A—N2A—C2A—N1A	0.3 (5)	N2B—C1B—C3B—C4B	−179.0 (8)
C3A—N1A—C2A—N2A	−0.1 (5)	N1B—C3B—C4B—C5B	60.4 (11)
N2A—C1A—C3A—N1A	0.3 (4)	C1B—C3B—C4B—C5B	−121.6 (10)
N2A—C1A—C3A—C4A	179.0 (4)	C3B—C4B—C5B—N3B	58.8 (9)
C2A—N1A—C3A—C1A	−0.1 (4)	C2BA—N2BA—C1BA—C3BA	−2 (4)
C2A—N1A—C3A—C4A	−178.9 (4)	C1BA—N2BA—C2BA—N1BA	−2 (3)
C1A—C3A—C4A—C5A	118.7 (5)	C3BA—N1BA—C2BA—N2BA	4 (2)
N1A—C3A—C4A—C5A	−62.9 (5)	C2BA—N1BA—C3BA—C1BA	−5 (3)
C3A—C4A—C5A—N3A	−64.0 (5)	C2BA—N1BA—C3BA—C4BA	174 (2)
C2B—N2B—C1B—C3B	0.9 (9)	N2BA—C1BA—C3BA—N1BA	4 (3)
C3B—N1B—C2B—N2B	0.3 (9)	N2BA—C1BA—C3BA—C4BA	−175 (2)
C1B—N2B—C2B—N1B	−0.7 (8)	N1BA—C3BA—C4BA—C5BA	−42 (3)
C2B—N1B—C3B—C1B	0.2 (10)	C1BA—C3BA—C4BA—C5BA	137 (3)
C2B—N1B—C3B—C4B	178.7 (7)	C3BA—C4BA—C5BA—N3BA	−50 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1*A*—H1*A*···O13^{i}	0.88	2.50	3.337 (4)	160
N1*A*—H1*A*···O14^{i}	0.88	2.49	3.052 (4)	122
N1*A*—H1*A*···O43^{ii}	0.88	2.47	3.021 (7)	121
N1*A*—H1*A*···O41*A*^{ii}	0.88	2.36	2.978 (9)	127
N2*A*—H2*A*···Cl4	0.88	2.96	3.709 (3)	145
N2*A*—H2*A*···O41	0.88	2.03	2.907 (9)	171
N2*A*—H2*A*···O44*A*	0.88	2.08	2.95 (2)	168
N3*A*—H3*A*1···O21^{iii}	0.91	2.56	3.040 (4)	114
N3*A*—H3*A*1···O34^{iv}	0.91	2.23	3.065 (6)	153
N3*A*—H3*A*1···O33*A*^{iv}	0.91	2.11	2.861 (12)	139
N3*A*—H3*A*2···Cl1^{v}	0.91	2.98	3.742 (3)	143
N3*A*—H3*A*2···O11^{v}	0.91	2.45	3.031 (4)	122

N3*A*—H3*A*2···O12^{v}	0.91	2.44	3.232 (4)	146
N3*A*—H3*A*2···O42^{v}	0.91	2.53	3.207 (8)	131
N3*A*—H3*A*2···O42*A*^{v}	0.91	2.57	3.272 (14)	134
N3*A*—H3*A*3···Cl3	0.91	2.95	3.735 (3)	145
N3*A*—H3*A*3···O31	0.91	2.51	3.055 (8)	119
N3*A*—H3*A*3···O32	0.91	2.26	3.120 (8)	159
N3*A*—H3*A*3···O32*A*	0.91	2.14	3.04 (2)	170
C2*A*—H2*AA*···O14^{i}	0.95	2.65	3.129 (5)	112
C2*A*—H2*AA*···O22	0.95	2.40	3.074 (5)	128
C4*A*—H4*AB*···O43^{ii}	0.99	2.66	3.379 (8)	129
C5*A*—H5*AA*···O42^{v}	0.99	2.70	3.158 (9)	109
C5*A*—H5*AA*···O43^{v}	0.99	2.70	3.310 (7)	120
C5*A*—H5*AB*···O12^{vi}	0.99	2.61	3.542 (5)	158
N1*B*—H1*B*···Cl1	0.88	2.91	3.714 (5)	153
N1*B*—H1*B*···O12	0.88	2.39	3.265 (6)	171
N1*B*—H1*B*···O14	0.88	2.38	2.961 (6)	124
N2*B*—H2*B*···O32	0.88	2.10	2.939 (9)	159
N3*B*—H3*B*1···Cl4	0.91	2.94	3.695 (14)	142
N3*B*—H3*B*1···O41	0.91	2.05	2.937 (19)	163
N3*B*—H3*B*1···O42	0.91	2.65	3.168 (13)	117
N3*B*—H3*B*2···O11^{vii}	0.91	2.56	3.120 (14)	120
N3*B*—H3*B*2···O13^{vii}	0.91	2.45	3.269 (11)	150
N3*B*—H3*B*2···O31^{viii}	0.91	2.63	3.310 (14)	132
N3*B*—H3*B*3···O21	0.91	2.36	2.910 (10)	119
N3*B*—H3*B*3···O34^{ix}	0.91	2.56	3.374 (13)	150
C1*B*—H1*BA*···O24^{ix}	0.95	2.64	3.441 (7)	142
C2*B*—H2*BA*···O22^{iii}	0.95	2.50	3.024 (6)	115
C4*B*—H4*BB*···O33^{ix}	0.99	2.50	3.433 (8)	156
C5*B*—H5*BA*···O11^{x}	0.99	2.52	3.249 (10)	130
N2*BA*—H2*B*1···O22^{iii}	0.88	2.38	3.150 (15)	146
N3*BA*—H3*B*4···Cl1^{vii}	0.91	2.78	3.62 (3)	155
N3*BA*—H3*B*4···O11^{vii}	0.91	2.15	2.93 (4)	144
N3*BA*—H3*B*4···O13^{vii}	0.91	2.40	3.12 (3)	137
N3*BA*—H3*B*4···O31*A*^{viii}	0.91	2.59	3.14 (4)	120
N3*BA*—H3*B*5···Cl2	0.91	2.82	3.66 (3)	154
N3*BA*—H3*B*5···O21	0.91	2.13	2.83 (2)	133
N3*BA*—H3*B*5···O24	0.91	2.48	3.29 (4)	149
N3*BA*—H3*B*6···Cl4	0.91	2.87	3.77 (4)	168
N3*BA*—H3*B*6···O44*A*	0.91	2.28	3.07 (5)	146
C1*BA*—H1*BB*···O14	0.95	2.16	3.103 (17)	171
C2*BA*—H2*BB*···Cl3	0.95	2.75	3.644 (14)	157
C2*BA*—H2*BB*···O32*A*	0.95	2.46	3.12 (3)	127
C2*BA*—H2*BB*···O34*A*	0.95	2.09	3.04 (2)	173
C4*BA*—H4*BD*···O11^{x}	0.99	2.56	3.250 (13)	127
C4*BA*—H4*BC*···O12	0.99	2.38	3.325 (16)	159
C5*BA*—H5*BC*···Cl3^{ix}	0.99	2.98	3.86 (3)	149

C5*BA*—H5*BC*···O34*A*^{ix}	0.99	2.26	3.18 (4)	153
C5*BA*—H5*BD*···O31*A*^{viii}	0.99	2.57	3.22 (4)	123

Symmetry codes: (i) −*x*+1, *y*−1/2, −*z*+1/2; (ii) −*x*+1, −*y*+1, −*z*+1; (iii) −*x*+1, *y*+1/2, −*z*+1/2; (iv) *x*, −*y*+3/2, *z*+1/2; (v) *x*−1, *y*, *z*; (vi) *x*−1, −*y*+3/2, *z*+1/2; (vii) −*x*+2, *y*−1/2, −*z*+1/2; (viii) *x*+1, *y*, *z*; (ix) −*x*+1, −*y*+1, −*z*; (x) *x*, −*y*+3/2, *z*−1/2.