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## Structure Reports

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## 2-[[2-(Piperazin-4-ium-1-yl)ethyl-iminio]methyl]phenolate 0.06-chloride 0.94-perchlorate

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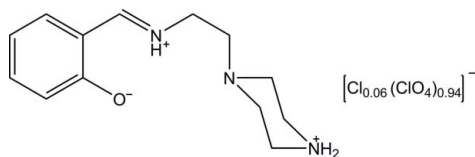
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Key indicators: single-crystal X-ray study;  $T = 100$  K; mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å; disorder in solvent or counterion;  $R$  factor = 0.045;  $wR$  factor = 0.127; data-to-parameter ratio = 13.4.

The structure of the title salt,  $\text{C}_{13}\text{H}_{20}\text{N}_3\text{O}^+ \cdot 0.94\text{ClO}_4^- \cdot 0.06\text{Cl}^-$ , contains a zwitterionic Schiff base with a net positive charge and a perchlorate anion having substitutional disorder with Cl. In the cation, the azomethine N atom is protonated and donates hydrogen bonds to the phenolate O atom and to the tertiary N atom of the piperazine ring. In the crystal, two Schiff base molecules are linked about a center of inversion by a pair of  $\text{N}-\text{H} \cdots \text{O}$  hydrogen bonds. The resulting dimers are  $\text{N}-\text{H} \cdots \text{O}$  and  $\text{C}-\text{H} \cdots \text{O}$  hydrogen bonded to the perchlorate anions, forming a three-dimensional structure. The network is further consolidated by  $\text{C}-\text{H} \cdots \pi$  interactions.

### Related literature

For the structure of a nickel(II) complex of the ligand, see: Mukhopadhyay *et al.* (2003). For the structure of a cadmium(II) complex of the ligand, see: Saleh Salga *et al.* (2010).



### Experimental

#### Crystal data

 $\text{C}_{13}\text{H}_{20}\text{N}_3\text{O}^+ \cdot 0.94\text{ClO}_4^- \cdot 0.06\text{Cl}^-$  $M_r = 329.74$ Monoclinic,  $P2_1/c$  $a = 11.2322$  (2) Å $b = 6.5240$  (1) Å $c = 21.0087$  (4) Å $\beta = 90.597$  (1)° $V = 1539.41$  (5) Å<sup>3</sup> $Z = 4$ Mo  $K\alpha$  radiation $\mu = 0.27$  mm<sup>-1</sup>  
 $T = 100$  K $0.28 \times 0.22 \times 0.18$  mm

#### Data collection

Bruker APEXII CCD  
diffractometerAbsorption correction: multi-scan  
(*SADABS*; Sheldrick, 1996)  
 $T_{\min} = 0.927$ ,  $T_{\max} = 0.952$ 11909 measured reflections  
2860 independent reflections  
2393 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.031$ 

#### Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.045$  $wR(F^2) = 0.127$  $S = 1.04$ 

2860 reflections

213 parameters

6 restraints

H atoms treated by a mixture of  
independent and constrained  
refinement $\Delta\rho_{\text{max}} = 0.58$  e Å<sup>-3</sup> $\Delta\rho_{\text{min}} = -0.27$  e Å<sup>-3</sup>

**Table 1**

Hydrogen-bond geometry (Å, °).

Cg1 is the centroid of the C1–C6 ring.

$D-\text{H} \cdots A$	$D-\text{H}$	$\text{H} \cdots A$	$D \cdots A$	$D-\text{H} \cdots A$
$\text{N1}-\text{H1} \cdots \text{O1}$	0.88 (3)	1.92 (3)	2.622 (2)	136 (2)
$\text{N1}-\text{H1} \cdots \text{N2}$	0.88 (3)	2.59 (3)	2.893 (3)	100.9 (19)
$\text{N3}-\text{H3A} \cdots \text{O4}^i$	0.86 (3)	2.23 (3)	3.020 (3)	153 (2)
$\text{N3}-\text{H3A} \cdots \text{O5}^i$	0.86 (3)	2.55 (3)	3.325 (3)	149 (2)
$\text{N3}-\text{H3B} \cdots \text{O1}^{ii}$	0.96 (3)	1.64 (3)	2.589 (2)	176 (2)
$\text{C5}-\text{H5} \cdots \text{O5}^{iii}$	0.95	2.43	3.217 (3)	140
$\text{C7}-\text{H7} \cdots \text{O3}^{iv}$	0.95	2.49	3.295 (3)	142
$\text{C9}-\text{H9B} \cdots \text{O2}^v$	0.99	2.47	3.271 (4)	138
$\text{C13}-\text{H13A} \cdots \text{O5}^i$	0.99	2.59	3.423 (4)	142
$\text{C13}-\text{H13B} \cdots \text{O4}^{vi}$	0.99	2.57	3.263 (3)	127
$\text{C3}-\text{H3} \cdots \text{Cg1}^{vii}$	0.95	2.70	3.500 (3)	142
$\text{C8}-\text{H8A} \cdots \text{Cg1}^v$	0.99	2.99	3.849 (3)	145

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

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: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008) and *pubCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PV2459).

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## supporting information

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## 2-[[2-(Piperazin-4-ium-1-yl)ethyliminio]methyl]phenolate 0.06-chloride 0.94-perchlorate

Mohammad Reza Reisi, Hamid Khaledi and Hapipah Mohd Ali

### S1. Comment

The Schiff base, 1-(2-salicylaldiminoethyl)piperazine, has been shown to exhibit different ligation behavior towards metal ions, mainly depending on the conformation adopted by the piperazine ring (Mukhopadhyay *et al.*, 2003; Saleh Salga *et al.*, 2010). In an attempt to prepare a tin(IV) complex of the Schiff base, the crystals of the title ion-pair were obtained unexpectedly. The Schiff base component is doubly protonated at its azomethine nitrogen, N1, and its secondary N atoms, N3, while being deprotonated at its oxygen atom, O1. The phenolate O1 atom is hydrogen bond acceptor from the protonated N1 and also from the N3 of a symmetry related molecule, forming a centrosymmetric dimer. The dimers are N—H $\cdots$ O and C—H $\cdots$ O bonded to the perchlorate anions to construct a three-dimensional polymeric structure. The network is further stabilized by C—H $\cdots$  $\pi$  interactions (Table 1). The anionic part is mainly perchlorate ion which displays small substitutional disorder with Cl [the site-occupancy factor of the perchlorate = 0.937 (2)].

### S2. Experimental

A mixture of salicylaldehyde (0.24 g, 2 mmol) and 4-(2-aminoethyl)piperazine (0.26 g, 2 mmol) in ethanol was refluxed for 2 h. Bu<sub>2</sub>SnCl<sub>2</sub> (0.6 g, 2 mmol) was then added and reflux was continued for another 2 h. The solution was cooled to room temperature and NaClO<sub>4</sub> (0.14 g, 1 mmol) was added to the mixture. The precipitated NaCl was separated out and the filtrate was evaporated under vacuum. The residue was dissolved in dichloromethane and left at room temperature for a day whereupon the brown crystals of the title compound were formed.

### S3. Refinement

The C-bound H atoms were placed at calculated positions and were treated as riding on their parent C atoms with H—C<sub>sp<sup>2</sup></sub> = 0.95 Å and H—C<sub>methylene</sub> = 0.99 Å. The N-bound H atoms were located in a difference Fourier map. For all H atoms, U<sub>iso</sub>(H) was set to 1.2U<sub>eq</sub>(carrier atom). An ISOR restraint (Sheldrick, 2008) was applied to a perchlorate oxygen atom, O3.

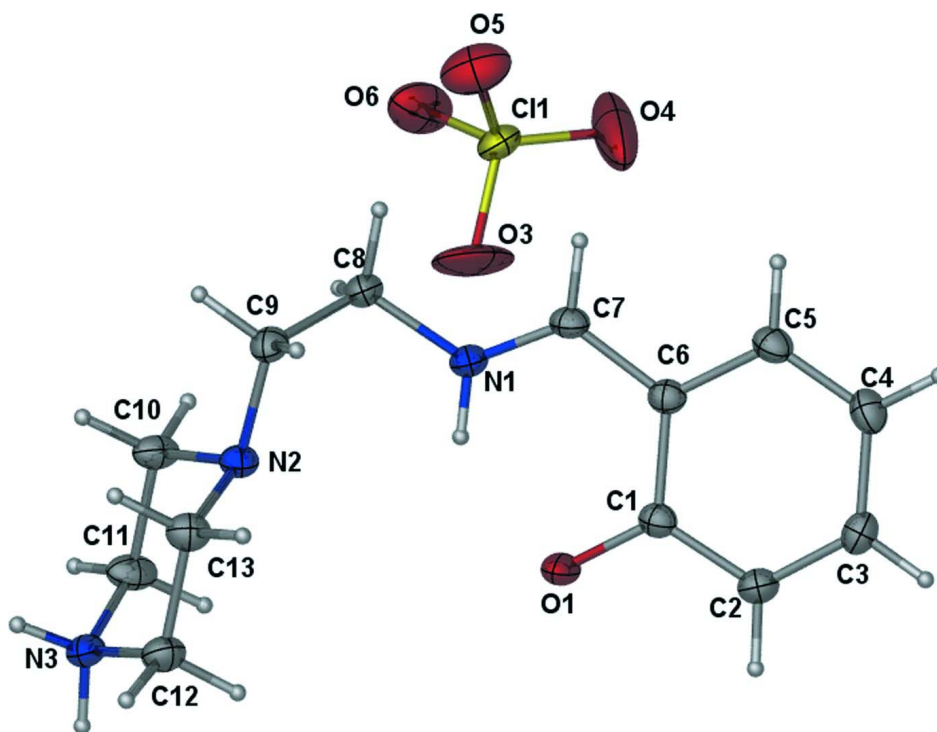


Figure 1

Molecular structure of the title compound with displacement ellipsoids at the 50% probability level. Hydrogen atoms are drawn as spheres of arbitrary radius. The partially occupying chloride ion is not depicted.

## 2-[[2-(Piperazin-4-ium-1-yl)ethyliminio]methyl]phenolate 0.06-chloride 0.94-perchlorate

### Crystal data

$C_{13}H_{20}N_3O^+ \cdot 0.94ClO_4^- \cdot 0.06Cl^-$

$M_r = 329.74$

Monoclinic,  $P2_1/c$

Hall symbol:  $-P\ 2ybc$

$a = 11.2322(2)\ \text{\AA}$

$b = 6.5240(1)\ \text{\AA}$

$c = 21.0087(4)\ \text{\AA}$

$\beta = 90.597(1)^\circ$

$V = 1539.41(5)\ \text{\AA}^3$

$Z = 4$

$F(000) = 696$

$D_x = 1.423\ \text{Mg m}^{-3}$

Mo  $K\alpha$  radiation,  $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 3417 reflections

$\theta = 2.7\text{--}29.0^\circ$

$\mu = 0.27\ \text{mm}^{-1}$

$T = 100\ \text{K}$

Block, brown

$0.28 \times 0.22 \times 0.18\ \text{mm}$

### Data collection

Bruker APEXII CCD  
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

$\varphi$  and  $\omega$  scans

Absorption correction: multi-scan  
(*SADABS*; Sheldrick, 1996)

$T_{\min} = 0.927$ ,  $T_{\max} = 0.952$

11909 measured reflections

2860 independent reflections

2393 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.031$

$\theta_{\max} = 25.5^\circ$ ,  $\theta_{\min} = 1.8^\circ$

$h = -13 \rightarrow 13$

$k = -7 \rightarrow 7$

$l = -24 \rightarrow 25$

Refinement

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.045$   
 $wR(F^2) = 0.127$   
 $S = 1.04$   
 2860 reflections  
 213 parameters  
 6 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  
 $w = 1/[\sigma^2(F_o^2) + (0.0613P)^2 + 1.4958P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.001$   
 $\Delta\rho_{\max} = 0.58 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\min} = -0.27 \text{ e } \text{\AA}^{-3}$

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 ( $\text{\AA}^2$ )

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
O1	0.92876 (14)	0.3289 (3)	0.88619 (8)	0.0288 (4)	
N1	0.72796 (16)	0.1530 (3)	0.85235 (9)	0.0241 (4)	
H1	0.793 (2)	0.153 (4)	0.8761 (12)	0.029*	
N2	0.72451 (16)	-0.0667 (3)	0.97192 (9)	0.0227 (4)	
N3	0.85668 (19)	-0.2651 (3)	1.07210 (10)	0.0279 (5)	
H3A	0.802 (3)	-0.323 (4)	1.0941 (13)	0.033*	
H3B	0.934 (2)	-0.290 (4)	1.0894 (12)	0.033*	
C1	0.90467 (19)	0.4724 (4)	0.84465 (10)	0.0232 (5)	
C2	0.9791 (2)	0.6457 (4)	0.83660 (11)	0.0258 (5)	
H2	1.0491	0.6584	0.8620	0.031*	
C3	0.9523 (2)	0.7957 (4)	0.79292 (11)	0.0265 (5)	
H3	1.0041	0.9099	0.7888	0.032*	
C4	0.8498 (2)	0.7835 (4)	0.75421 (11)	0.0285 (5)	
H4	0.8325	0.8877	0.7239	0.034*	
C5	0.7754 (2)	0.6190 (4)	0.76094 (11)	0.0258 (5)	
H5	0.7057	0.6100	0.7351	0.031*	
C6	0.80000 (19)	0.4627 (3)	0.80549 (10)	0.0224 (5)	
C7	0.71557 (19)	0.3007 (4)	0.81201 (10)	0.0233 (5)	
H7	0.6468	0.3017	0.7853	0.028*	
C8	0.6394 (2)	-0.0046 (4)	0.86529 (11)	0.0267 (5)	
H8A	0.6691	-0.1401	0.8514	0.032*	
H8B	0.5648	0.0255	0.8416	0.032*	
C9	0.61617 (19)	-0.0068 (4)	0.93633 (11)	0.0253 (5)	
H9A	0.5904	0.1311	0.9502	0.030*	

H9B	0.5513	-0.1047	0.9456	0.030*	
C10	0.7358 (2)	-0.2908 (4)	0.97354 (12)	0.0279 (5)	
H10A	0.7346	-0.3456	0.9296	0.034*	
H10B	0.6678	-0.3507	0.9967	0.034*	
C11	0.8518 (2)	-0.3499 (4)	1.00654 (12)	0.0317 (6)	
H11A	0.8584	-0.5011	1.0083	0.038*	
H11B	0.9197	-0.2968	0.9818	0.038*	
C12	0.8353 (2)	-0.0404 (4)	1.07244 (12)	0.0284 (5)	
H12A	0.9028	0.0304	1.0520	0.034*	
H12B	0.8303	0.0085	1.1169	0.034*	
C13	0.7209 (2)	0.0115 (4)	1.03721 (11)	0.0274 (5)	
H13A	0.6525	-0.0499	1.0597	0.033*	
H13B	0.7099	0.1620	1.0365	0.033*	
Cl1	0.40865 (5)	0.51801 (10)	0.85512 (4)	0.0300 (2)	0.937 (3)
O2	0.4847 (3)	0.5543 (5)	0.90856 (15)	0.0754 (9)	0.937 (3)
O3	0.4569 (2)	0.6021 (6)	0.79982 (15)	0.0915 (11)	0.937 (3)
O4	0.29220 (18)	0.5955 (4)	0.86711 (11)	0.0508 (6)	0.937 (3)
O5	0.3970 (2)	0.3003 (3)	0.84855 (11)	0.0556 (7)	0.937 (3)
Cl2	0.4427 (11)	0.4812 (19)	0.8918 (7)	0.035 (4)*	0.063 (3)

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
O1	0.0230 (8)	0.0290 (9)	0.0341 (9)	-0.0034 (7)	-0.0090 (7)	0.0078 (7)
N1	0.0182 (9)	0.0287 (11)	0.0252 (10)	-0.0029 (8)	-0.0033 (8)	0.0015 (8)
N2	0.0191 (9)	0.0236 (10)	0.0254 (10)	0.0013 (8)	-0.0021 (7)	-0.0009 (8)
N3	0.0203 (10)	0.0295 (11)	0.0337 (11)	-0.0054 (8)	-0.0065 (8)	0.0061 (9)
C1	0.0221 (11)	0.0261 (12)	0.0214 (11)	0.0016 (9)	0.0008 (9)	-0.0008 (9)
C2	0.0220 (11)	0.0283 (12)	0.0272 (12)	-0.0016 (9)	-0.0020 (9)	-0.0022 (10)
C3	0.0262 (12)	0.0237 (12)	0.0298 (12)	-0.0021 (9)	0.0064 (9)	-0.0006 (10)
C4	0.0308 (12)	0.0282 (13)	0.0266 (12)	0.0055 (10)	0.0044 (10)	0.0048 (10)
C5	0.0215 (11)	0.0314 (13)	0.0244 (12)	0.0042 (9)	-0.0012 (9)	0.0009 (10)
C6	0.0205 (11)	0.0247 (12)	0.0222 (11)	0.0018 (9)	0.0008 (9)	-0.0022 (9)
C7	0.0184 (10)	0.0292 (12)	0.0223 (11)	0.0021 (9)	-0.0021 (8)	-0.0012 (9)
C8	0.0220 (11)	0.0292 (13)	0.0289 (12)	-0.0053 (9)	-0.0034 (9)	0.0027 (10)
C9	0.0187 (11)	0.0267 (12)	0.0305 (13)	0.0009 (9)	0.0003 (9)	0.0025 (10)
C10	0.0253 (12)	0.0249 (12)	0.0334 (13)	0.0015 (9)	-0.0079 (10)	-0.0040 (10)
C11	0.0291 (12)	0.0253 (13)	0.0406 (14)	0.0053 (10)	-0.0108 (11)	-0.0044 (11)
C12	0.0259 (12)	0.0278 (13)	0.0315 (13)	-0.0027 (10)	-0.0035 (10)	-0.0037 (10)
C13	0.0260 (12)	0.0270 (12)	0.0293 (13)	0.0024 (9)	-0.0014 (10)	-0.0039 (10)
Cl1	0.0209 (3)	0.0334 (4)	0.0357 (5)	-0.0080 (2)	-0.0022 (3)	-0.0010 (3)
O2	0.0628 (17)	0.0668 (17)	0.095 (2)	-0.0180 (14)	-0.0517 (16)	-0.0201 (16)
O3	0.0471 (15)	0.134 (3)	0.094 (2)	0.0135 (16)	0.0184 (14)	0.080 (2)
O4	0.0304 (11)	0.0582 (14)	0.0639 (15)	0.0050 (10)	0.0055 (10)	-0.0243 (12)
O5	0.0702 (16)	0.0310 (12)	0.0651 (15)	-0.0043 (11)	-0.0238 (12)	-0.0091 (10)

*Geometric parameters (Å, °)*

O1—C1	1.306 (3)	C6—C7	1.427 (3)
N1—C7	1.290 (3)	C7—H7	0.9500
N1—C8	1.458 (3)	C8—C9	1.518 (3)
N1—H1	0.88 (3)	C8—H8A	0.9900
N2—C13	1.464 (3)	C8—H8B	0.9900
N2—C10	1.468 (3)	C9—H9A	0.9900
N2—C9	1.474 (3)	C9—H9B	0.9900
N3—C11	1.485 (3)	C10—C11	1.519 (3)
N3—C12	1.485 (3)	C10—H10A	0.9900
N3—H3A	0.86 (3)	C10—H10B	0.9900
N3—H3B	0.96 (3)	C11—H11A	0.9900
C1—C2	1.417 (3)	C11—H11B	0.9900
C1—C6	1.429 (3)	C12—C13	1.514 (3)
C2—C3	1.373 (3)	C12—H12A	0.9900
C2—H2	0.9500	C12—H12B	0.9900
C3—C4	1.405 (3)	C13—H13A	0.9900
C3—H3	0.9500	C13—H13B	0.9900
C4—C5	1.369 (3)	C11—O3	1.399 (3)
C4—H4	0.9500	C11—O2	1.424 (3)
C5—C6	1.410 (3)	C11—O4	1.427 (2)
C5—H5	0.9500	C11—O5	1.433 (2)
C7—N1—C8	125.5 (2)	H8A—C8—H8B	108.4
C7—N1—H1	117.1 (17)	N2—C9—C8	110.59 (18)
C8—N1—H1	117.3 (17)	N2—C9—H9A	109.5
C13—N2—C10	109.16 (18)	C8—C9—H9A	109.5
C13—N2—C9	110.63 (17)	N2—C9—H9B	109.5
C10—N2—C9	110.26 (17)	C8—C9—H9B	109.5
C11—N3—C12	111.59 (19)	H9A—C9—H9B	108.1
C11—N3—H3A	108.3 (19)	N2—C10—C11	109.68 (19)
C12—N3—H3A	108.3 (18)	N2—C10—H10A	109.7
C11—N3—H3B	108.3 (16)	C11—C10—H10A	109.7
C12—N3—H3B	108.3 (16)	N2—C10—H10B	109.7
H3A—N3—H3B	112 (2)	C11—C10—H10B	109.7
O1—C1—C2	122.2 (2)	H10A—C10—H10B	108.2
O1—C1—C6	121.1 (2)	N3—C11—C10	110.6 (2)
C2—C1—C6	116.7 (2)	N3—C11—H11A	109.5
C3—C2—C1	121.5 (2)	C10—C11—H11A	109.5
C3—C2—H2	119.2	N3—C11—H11B	109.5
C1—C2—H2	119.2	C10—C11—H11B	109.5
C2—C3—C4	121.3 (2)	H11A—C11—H11B	108.1
C2—C3—H3	119.3	N3—C12—C13	110.77 (19)
C4—C3—H3	119.3	N3—C12—H12A	109.5
C5—C4—C3	118.8 (2)	C13—C12—H12A	109.5
C5—C4—H4	120.6	N3—C12—H12B	109.5
C3—C4—H4	120.6	C13—C12—H12B	109.5

C4—C5—C6	121.3 (2)	H12A—C12—H12B	108.1
C4—C5—H5	119.3	N2—C13—C12	110.40 (19)
C6—C5—H5	119.3	N2—C13—H13A	109.6
C5—C6—C7	118.2 (2)	C12—C13—H13A	109.6
C5—C6—C1	120.3 (2)	N2—C13—H13B	109.6
C7—C6—C1	121.4 (2)	C12—C13—H13B	109.6
N1—C7—C6	123.3 (2)	H13A—C13—H13B	108.1
N1—C7—H7	118.4	O3—C11—O2	110.8 (2)
C6—C7—H7	118.4	O3—C11—O4	111.81 (16)
N1—C8—C9	108.35 (19)	O2—C11—O4	110.21 (16)
N1—C8—H8A	110.0	O3—C11—O5	110.2 (2)
C9—C8—H8A	110.0	O2—C11—O5	107.10 (16)
N1—C8—H8B	110.0	O4—C11—O5	106.59 (15)
C9—C8—H8B	110.0		

*Hydrogen-bond geometry (Å, °)*

Cg1 is the centroid of the C1—C6 ring.

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
N1—H1 $\cdots$ O1	0.88 (3)	1.92 (3)	2.622 (2)	136 (2)
N1—H1 $\cdots$ N2	0.88 (3)	2.59 (3)	2.893 (3)	100.9 (19)
N3—H3A $\cdots$ O4 <sup>i</sup>	0.86 (3)	2.23 (3)	3.020 (3)	153 (2)
N3—H3A $\cdots$ O5 <sup>i</sup>	0.86 (3)	2.55 (3)	3.325 (3)	149 (2)
N3—H3B $\cdots$ O1 <sup>ii</sup>	0.96 (3)	1.64 (3)	2.589 (2)	176 (2)
C5—H5 $\cdots$ O5 <sup>iii</sup>	0.95	2.43	3.217 (3)	140
C7—H7 $\cdots$ O3 <sup>iv</sup>	0.95	2.49	3.295 (3)	142
C9—H9B $\cdots$ O2 <sup>v</sup>	0.99	2.47	3.271 (4)	138
C13—H13A $\cdots$ O5 <sup>i</sup>	0.99	2.59	3.423 (4)	142
C13—H13B $\cdots$ O4 <sup>vi</sup>	0.99	2.57	3.263 (3)	127
C3—H3 $\cdots$ Cg1 <sup>vii</sup>	0.95	2.70	3.500 (3)	142
C8—H8A $\cdots$ Cg1 <sup>v</sup>	0.99	2.99	3.849 (3)	145

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