Crystal structure of 4-*tert*-butyl-2-{2-[*N*-(3,3-dimethyl-2-oxobutyl)-*N*-isopropylcarbamoyl]-phenyl}-1-isopropyl-1*H*-imidazol-3-ium perchlorate

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In the title salt, $C_{26}H_{40}N_3O_2{}^+ \cdot ClO_4{}^-$, the positive charge of the organic cation is delocalized between the two N atoms of the imidazole ring. The C⋯N bond distances are 1.338 (2) and 1.327 (3) Å. The substituents on the benzene ring are rotated almost orthogonal with respect to this ring due to the presence of the bulky isopropyl substituents. The dihedral angle between the benzene and imidazole rings is 75.15 (12)°. Three of the O atoms of the anion are disordered over two sets of sites due to rotation around one of the O—Cl bonds. The ratio of the refined occupancies is 0.591 (14):0.409 (14). In the crystal, the cation and perchlorate anion are bound by an N—H⋯O hydrogen bond. In addition, the cation–anion pairs are linked into layers parallel to (001) by multiple weak C—H⋯O hydrogen bonds.

1. Chemical context

α-Aminoketones are known for their fungicidal activity (Gold de Sigman, 1983) and 2-acylaminoketones are the starting compounds in the oxazole synthetic method by the Robinson–Gabriel synthesis by dehydration of 2-acylaminoketones (Robinson, 1909; Gabriel, 1910; Wasserman & Vinick, 1973) that has been used during studies dealing with pharmaceutically important molecules that incorporate an oxazole derivative (Godfrey *et al.*, 2003; Nicolaou *et al.*, 2004; Hoffman *et al.*, 2010).
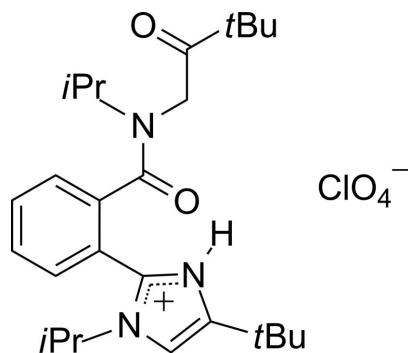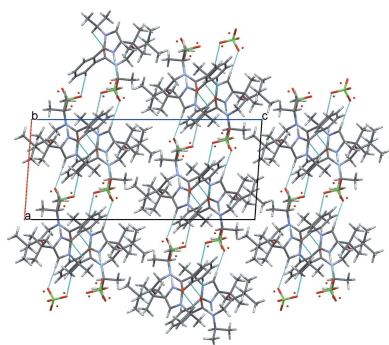
2. Structural commentary

The molecular structure of the cation is shown in Fig. 1. The positive charge is delocalized between the two nitrogen atoms of the imidazole ring according to almost equivalent lengths of the C7—N1 and C7—N2 bonds [1.338 (2) Å and 1.327 (3) Å, respectively] and also of the C8—N1 and C9—N2 bonds [1.379 (3) Å and 1.374 (3) Å, respectively]. The presence of
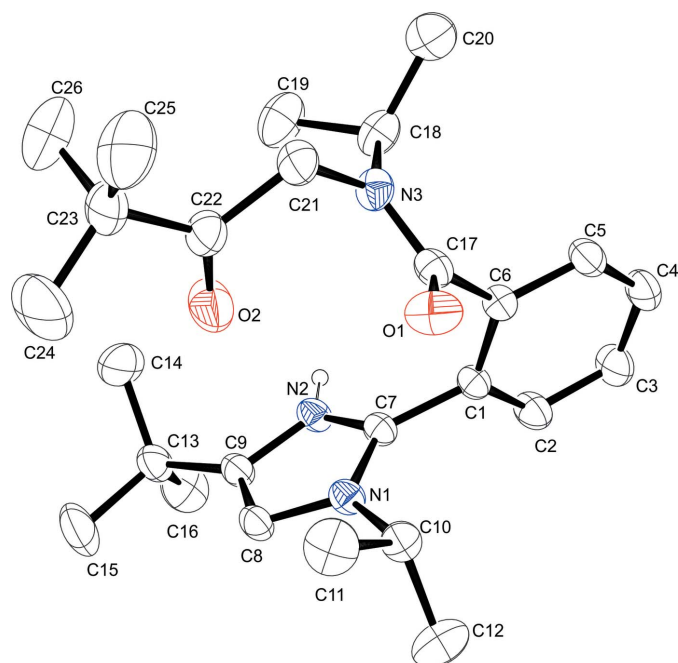
Figure 1
View of the title compound showing the atom-numbering scheme and 30% probability displacement ellipsoids. For clarity, the ClO$_4^-$ anion and H atoms are not shown.

two bulky substituents in the *ortho* positions of the benzene ring results in disruption of the conjugation between the aromatic ring, imidazole ring and amide [N3/C17/O1] fragment due to their almost orthogonal orientation [the corresponding torsion angles are N1—C7—C1—C6 = −81.5 (3)° and C5—C6—C17—N3 = 81.1 (3)°]. The plane of the carbonyl group (C22/O2/C23/C21) is oriented almost orthogonal to the

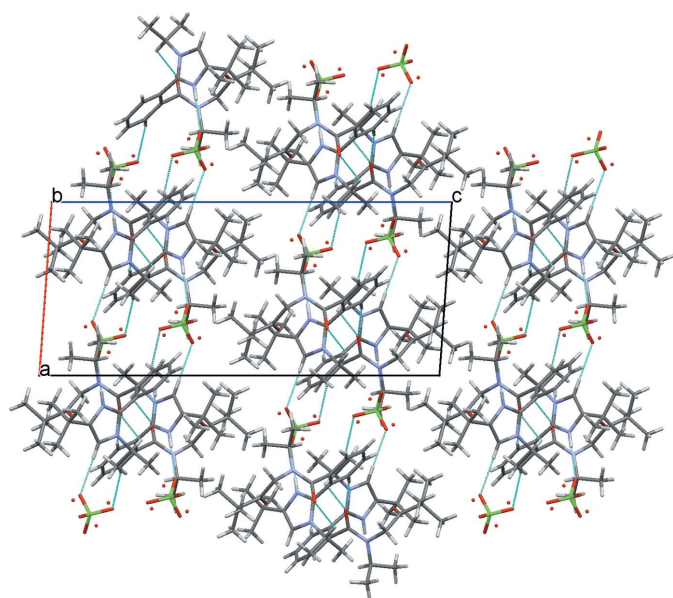**Figure 2**
Part of the crystal structure, viewed along the *b* axis, showing layers parallel to (001) formed by weak C—H⋯O hydrogen bonds (turquoise dotted lines) and also separated layers of organic cations parallel to (101). The minor disorder component of the anion is shown as red spheres.

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
N2—H2⋯O3	0.86	1.94	2.752 (4)	157
C2—H2A⋯O1^i	0.93	2.44	3.319 (3)	158
C5—H5⋯O5A^{ii}	0.93	2.55	3.328 (11)	141
C8—H8⋯O4A^{iii}	0.93	2.36	3.285 (8)	173

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

plane of the amide fragment (C21/N3/C18/C17/O1/C6), the angle between their mean planes being 77.87 (11)°. A similar type of α-acylaminoketone fragment has been observed for other *N*-substituted α-acylaminoketones (Bartnik *et al.*, 1998; Tinant *et al.*, 2006; Chai *et al.*, 2011; Hashmi *et al.*, 2011; Su *et al.*, 2011).

The organic cation and perchlorate anion are linked by an N—H⋯O hydrogen bond (Table 1). The oxygen atoms of the anion are disordered over two sets of sites due to rotation around the O3—Cl bond. The refined occupancy of the major disordered component is 0.591 (14).

3. Supramolecular features

Several moderate to weak C—H⋯O intermolecular hydrogen bonds are observed in the crystal structure (Table 1), which link molecules into layers parallel to (001) (Fig. 2). It should also be noted that the crystal structure contains no residual solvent-accessible voids. However, discernible layers along (101) are observed. The low density [1.18 g mm^{-1}] of the crystal could be associated with formation of these layers.

4. Synthesis and crystallization

The title compound was synthesized according to the literature procedure (Hordiyenko *et al.*, 2009). To a stirred solution of 1-(*N*-isopropylamino)-3,3-dimethylbutan-2-one (10 mmol) in dry CHCl$_3$ (10 mL), a solution of 1,1,3-trichloro-1*H*-isoindole (2.5 mmol) in dry CHCl$_3$ (10 mL) was added dropwise at room temperature under an argon atmosphere. The reaction mixture was stirred for 8 h, the solvent was evaporated and the residue was dried under reduced pressure (0.01 mm). Then it was treated with 100 ml of distilled water. The aqueous solution was brought to reflux with charcoal, filtered and treated with an excess of lithium perchlorate to precipitate the crude product that was then crystallized from methanol/water (3:1) to yield as colorless crystals. Single crystals suitable for X-ray diffraction were obtained by slow evaporation of a solution of the title compound in ethanol.

5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Hydrogen atoms were placed in calculated positions (N—H = 0.86 Å, C—H = 0.93–0.98 Å) and refined in a riding-model approximation with $U_{iso} = nU_{eq}$ of the carrier atom (n = 1.5 for methyl groups, n = 1.2 for the

Table 2
Experimental details.

Crystal data

Chemical formula	$C_{26}H_{40}N_3O_2{}^+\cdot ClO_4{}^-$
M_r	526.06
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	293
a, b, c (Å)	10.0605 (3), 12.7027 (4), 23.1455 (6)
β (°)	94.107 (3)
V (Å^3)	2950.29 (14)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.17
Crystal size (mm)	$0.57 \times 0.32 \times 0.09$

Data collection

Diffractometer	Agilent Xcalibur Sapphire3
Absorption correction	Multi-scan (*CrysAlis PRO*; Agilent, 2014)
T_{min}, T_{max}	0.951, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	27330, 6037, 4458
R_{int}	0.029
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.626

Refinement

$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.060, 0.179, 1.04
No. of reflections	6037
No. of parameters	363
No. of restraints	87
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å^{-3})	0.37, −0.33

Computer programs: *CrysAlis PRO* (Agilent, 2014), *SHELXD* (Sheldrick, 2008), *SHELXL97* (Sheldrick, 2015) and *OLEX2* (Dolomanov *et al.*, 2009).

remaining H atoms). Methyl groups were refined as rotating groups. The relative occupation of the two positions of the disordered ClO$_4$ anion was refined as a free variable. All Cl—

O and O⋯O distances within the anion were restrained to be the same within 0.02 Å.

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supporting information

Crystal structure of 4-*tert*-butyl-2-{2-[*N*-(3,3-dimethyl-2-oxobutyl)-*N*-isopropyl-carbamoyl]phenyl}-1-isopropyl-1*H*-imidazol-3-ium perchlorate

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Computing details

Data collection: *CrysAlis PRO* (Agilent, 2014); cell refinement: *CrysAlis PRO* (Agilent, 2014); data reduction: *CrysAlis PRO* (Agilent, 2014); program(s) used to solve structure: *SHELXD* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2015); molecular graphics: OLEX2 (Dolomanov *et al.*, 2009); software used to prepare material for publication: OLEX2 (Dolomanov *et al.*, 2009).

4-*tert*-Butyl-2-{2-[*N*-(3,3-dimethyl-2-oxobutyl)-*N*-isopropylcarbamoyl]phenyl}-1-isopropyl-1*H*-imidazol-3-ium perchlorate

Crystal data

$C_{26}H_{40}N_3O_2^+ \cdot ClO_4^-$	$F(000) = 1128$
$M_r = 526.06$	$D_x = 1.184$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 10.0605$ (3) Å	Cell parameters from 6208 reflections
$b = 12.7027$ (4) Å	$\theta = 3.2$–$26.2°$
$c = 23.1455$ (6) Å	$\mu = 0.17$ mm^{-1}
$\beta = 94.107$ (3)°	$T = 293$ K
$V = 2950.29$ (14) Å^3	Block, colorless
$Z = 4$	$0.57 \times 0.32 \times 0.09$ mm

Data collection

Agilent Xcalibur Sapphire3 diffractometer	27330 measured reflections
Radiation source: Enhance (Mo) X-ray Source	6037 independent reflections
Graphite monochromator	4458 reflections with $I > 2\sigma(I)$
Detector resolution: 16.1827 pixels mm^{-1}	$R_{int} = 0.029$
ω and π scans	$\theta_{max} = 26.4°$, $\theta_{min} = 3.1°$
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2014)	$h = -12 \rightarrow 12$
	$k = -15 \rightarrow 15$
	$l = -28 \rightarrow 28$
$T_{min} = 0.951$, $T_{max} = 1.000$	

Refinement

Refinement on F^2	87 restraints
Least-squares matrix: full	Primary atom site location: dual
$R[F^2 > 2\sigma(F^2)] = 0.060$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.179$	H-atom parameters constrained
$S = 1.04$	$w = 1/[\sigma^2(F_o^2) + (0.0837P)^2 + 1.4781P]$
6037 reflections	where $P = (F_o^2 + 2F_c^2)/3$
363 parameters	

$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.37$ e Å^{-3}

$\Delta\rho_{min} = -0.33$ 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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
O1	0.72746 (17)	0.14319 (15)	0.71062 (9)	0.0685 (5)	
O2	0.7339 (3)	0.25979 (17)	0.58916 (9)	0.0915 (7)	
N2	0.67413 (16)	0.47485 (14)	0.66538 (8)	0.0421 (4)	
H2	0.5935	0.4962	0.6583	0.051*	
N1	0.84449 (16)	0.39425 (14)	0.70494 (7)	0.0416 (4)	
C7	0.71299 (19)	0.40741 (15)	0.70699 (9)	0.0383 (4)	
C8	0.8863 (2)	0.45571 (18)	0.66063 (9)	0.0450 (5)	
H8	0.9735	0.4614	0.6501	0.054*	
C1	0.62173 (19)	0.36474 (16)	0.74861 (9)	0.0398 (4)	
C6	0.5700 (2)	0.26255 (16)	0.74384 (9)	0.0420 (5)	
C9	0.7801 (2)	0.50599 (18)	0.63519 (9)	0.0442 (5)	
N3	0.54488 (19)	0.17087 (15)	0.65053 (8)	0.0496 (5)	
C17	0.6201 (2)	0.18761 (16)	0.70018 (10)	0.0463 (5)	
C10	0.9309 (2)	0.32719 (18)	0.74425 (10)	0.0488 (5)	
H10	0.8739	0.2799	0.7650	0.059*	
C2	0.5770 (2)	0.43279 (19)	0.79004 (11)	0.0537 (6)	
H2A	0.6106	0.5009	0.7931	0.064*	
C5	0.4771 (2)	0.23065 (19)	0.78176 (10)	0.0538 (6)	
H5	0.4437	0.1624	0.7795	0.065*	
C4	0.4338 (3)	0.2986 (2)	0.82254 (11)	0.0609 (7)	
H4	0.3710	0.2763	0.8475	0.073*	
C21	0.6048 (3)	0.10861 (19)	0.60668 (11)	0.0570 (6)	
H21A	0.5351	0.0816	0.5795	0.068*	
H21B	0.6509	0.0490	0.6250	0.068*	
C13	0.7626 (2)	0.5776 (2)	0.58316 (11)	0.0566 (6)	
C3	0.4831 (3)	0.3996 (2)	0.82658 (11)	0.0625 (7)	
H3	0.4529	0.4456	0.8540	0.075*	
C22	0.7029 (3)	0.1726 (2)	0.57379 (11)	0.0625 (7)	
C18	0.4094 (3)	0.2141 (2)	0.63707 (11)	0.0592 (6)	
H18	0.3952	0.2695	0.6654	0.071*	
C11	1.0206 (3)	0.2608 (3)	0.70900 (14)	0.0773 (8)	
H11A	0.9682	0.2274	0.6779	0.116*	
H11B	1.0637	0.2080	0.7334	0.116*	
H11C	1.0867	0.3049	0.6934	0.116*	
C12	1.0089 (3)	0.3951 (3)	0.78810 (14)	0.0817 (9)	
H12A	1.0651	0.4422	0.7685	0.123*	
H12B	1.0630	0.3512	0.8141	0.123*	

H12C	0.9484	0.4351	0.8097	0.123*	
C14	0.6630 (4)	0.5257 (3)	0.53881 (14)	0.0929 (11)	
H14A	0.6956	0.4577	0.5286	0.139*	
H14B	0.6524	0.5689	0.5048	0.139*	
H14C	0.5786	0.5181	0.5552	0.139*	
C20	0.3049 (3)	0.1288 (3)	0.64423 (14)	0.0758 (8)	
H20A	0.3203	0.0711	0.6188	0.114*	
H20B	0.2177	0.1573	0.6348	0.114*	
H20C	0.3111	0.1045	0.6836	0.114*	
C16	0.7086 (4)	0.6841 (3)	0.60196 (16)	0.0877 (10)	
H16A	0.6257	0.6736	0.6193	0.132*	
H16B	0.6946	0.7291	0.5688	0.132*	
H16C	0.7717	0.7162	0.6296	0.132*	
C23	0.7609 (3)	0.1226 (3)	0.52116 (13)	0.0782 (9)	
C25	0.7743 (5)	0.0024 (3)	0.52725 (19)	0.1192 (15)	
H25A	0.8327	−0.0139	0.5607	0.179*	
H25B	0.8104	−0.0259	0.4933	0.179*	
H25C	0.6882	−0.0278	0.5316	0.179*	
C15	0.8972 (3)	0.5924 (3)	0.55791 (15)	0.0943 (11)	
H15A	0.9590	0.6232	0.5866	0.141*	
H15B	0.8870	0.6379	0.5248	0.141*	
H15C	0.9304	0.5253	0.5464	0.141*	
C19	0.3955 (4)	0.2640 (3)	0.57734 (13)	0.0843 (9)	
H19A	0.4649	0.3151	0.5741	0.127*	
H19B	0.3103	0.2980	0.5718	0.127*	
H19C	0.4024	0.2106	0.5484	0.127*	
C26	0.6614 (5)	0.1441 (4)	0.46941 (16)	0.1277 (16)	
H26A	0.5769	0.1131	0.4764	0.192*	
H26B	0.6939	0.1139	0.4351	0.192*	
H26C	0.6508	0.2187	0.4643	0.192*	
C24	0.8914 (5)	0.1763 (5)	0.5105 (3)	0.177 (3)	
H24A	0.8760	0.2501	0.5039	0.265*	
H24B	0.9277	0.1458	0.4771	0.265*	
H24C	0.9532	0.1671	0.5436	0.265*	
Cl1	0.29860 (6)	0.54707 (6)	0.65153 (4)	0.0755 (3)	
O3	0.4025 (3)	0.4841 (3)	0.64132 (19)	0.1626 (16)	
O4A	0.1909 (7)	0.4970 (13)	0.6233 (5)	0.233 (7)	0.591 (14)
O5A	0.2680 (11)	0.5578 (8)	0.7063 (3)	0.177 (5)	0.591 (14)
O6A	0.3130 (16)	0.6413 (6)	0.6273 (7)	0.276 (10)	0.591 (14)
O6B	0.3652 (14)	0.6383 (9)	0.6691 (8)	0.235 (10)	0.409 (14)
O4B	0.2175 (13)	0.5692 (15)	0.6066 (6)	0.216 (10)	0.409 (14)
O5B	0.2331 (17)	0.5113 (17)	0.6954 (8)	0.316 (17)	0.409 (14)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0517 (10)	0.0604 (11)	0.0927 (13)	0.0105 (8)	0.0006 (9)	−0.0208 (10)
O2	0.1285 (19)	0.0672 (13)	0.0840 (14)	−0.0322 (13)	0.0444 (13)	−0.0187 (11)

N2	0.0307 (8)	0.0455 (10)	0.0506 (10)	0.0019 (7)	0.0051 (7)	0.0055 (8)
N1	0.0334 (8)	0.0437 (9)	0.0480 (10)	0.0036 (7)	0.0054 (7)	0.0018 (8)
C7	0.0356 (10)	0.0363 (10)	0.0435 (10)	−0.0001 (8)	0.0072 (8)	−0.0008 (8)
C8	0.0339 (10)	0.0532 (12)	0.0489 (12)	−0.0025 (9)	0.0100 (8)	0.0042 (10)
C1	0.0357 (10)	0.0408 (11)	0.0437 (11)	0.0003 (8)	0.0075 (8)	0.0001 (9)
C6	0.0419 (11)	0.0407 (11)	0.0437 (11)	−0.0004 (8)	0.0062 (8)	0.0012 (9)
C9	0.0364 (10)	0.0496 (12)	0.0471 (11)	−0.0044 (9)	0.0064 (8)	0.0047 (9)
N3	0.0583 (11)	0.0440 (10)	0.0474 (10)	0.0052 (8)	0.0108 (8)	−0.0045 (8)
C17	0.0500 (12)	0.0341 (10)	0.0562 (13)	−0.0023 (9)	0.0129 (10)	−0.0007 (9)
C10	0.0425 (11)	0.0502 (13)	0.0532 (12)	0.0078 (9)	0.0003 (9)	0.0068 (10)
C2	0.0567 (14)	0.0449 (12)	0.0614 (14)	−0.0075 (10)	0.0185 (11)	−0.0092 (10)
C5	0.0567 (14)	0.0501 (13)	0.0561 (13)	−0.0130 (10)	0.0151 (11)	0.0002 (10)
C4	0.0593 (14)	0.0713 (17)	0.0550 (14)	−0.0132 (12)	0.0241 (11)	−0.0034 (12)
C21	0.0699 (16)	0.0465 (13)	0.0565 (14)	0.0007 (11)	0.0176 (12)	−0.0113 (11)
C13	0.0482 (13)	0.0664 (15)	0.0549 (13)	−0.0077 (11)	0.0015 (10)	0.0206 (12)
C3	0.0661 (16)	0.0669 (16)	0.0578 (14)	−0.0076 (13)	0.0273 (12)	−0.0159 (12)
C22	0.0750 (17)	0.0586 (16)	0.0553 (14)	−0.0039 (13)	0.0150 (12)	−0.0095 (12)
C18	0.0714 (16)	0.0542 (14)	0.0512 (13)	0.0172 (12)	−0.0007 (11)	−0.0072 (11)
C11	0.0663 (17)	0.0764 (19)	0.090 (2)	0.0317 (15)	0.0076 (15)	−0.0001 (16)
C12	0.085 (2)	0.079 (2)	0.0765 (19)	0.0132 (17)	−0.0260 (16)	−0.0101 (16)
C14	0.104 (3)	0.107 (3)	0.0633 (18)	−0.032 (2)	−0.0244 (17)	0.0306 (18)
C20	0.0575 (16)	0.087 (2)	0.083 (2)	0.0093 (14)	0.0054 (14)	−0.0102 (16)
C16	0.093 (2)	0.071 (2)	0.099 (2)	0.0079 (17)	0.0018 (18)	0.0326 (18)
C23	0.084 (2)	0.088 (2)	0.0668 (17)	−0.0032 (16)	0.0307 (15)	−0.0167 (15)
C25	0.150 (4)	0.109 (3)	0.103 (3)	0.036 (3)	0.042 (3)	−0.029 (2)
C15	0.0691 (19)	0.134 (3)	0.082 (2)	−0.0079 (19)	0.0244 (16)	0.048 (2)
C19	0.115 (3)	0.076 (2)	0.0605 (17)	0.0214 (18)	−0.0077 (16)	0.0058 (15)
C26	0.169 (4)	0.150 (4)	0.064 (2)	0.021 (3)	0.011 (2)	−0.016 (2)
C24	0.136 (4)	0.234 (7)	0.174 (5)	−0.073 (4)	0.105 (4)	−0.088 (5)
Cl1	0.0441 (4)	0.0817 (5)	0.1017 (6)	0.0188 (3)	0.0118 (3)	−0.0090 (4)
O3	0.0613 (15)	0.151 (3)	0.274 (5)	0.0386 (17)	0.002 (2)	−0.070 (3)
O4A	0.054 (3)	0.45 (2)	0.195 (10)	−0.068 (7)	0.005 (4)	−0.011 (11)
O5A	0.236 (12)	0.177 (8)	0.126 (6)	0.064 (8)	0.076 (6)	−0.025 (5)
O6A	0.38 (2)	0.108 (6)	0.37 (2)	0.114 (9)	0.229 (15)	0.112 (9)
O6B	0.272 (16)	0.184 (13)	0.248 (18)	−0.150 (12)	0.012 (13)	−0.095 (12)
O4B	0.089 (9)	0.35 (3)	0.194 (12)	0.039 (11)	−0.079 (9)	0.058 (14)
O5B	0.179 (14)	0.45 (3)	0.33 (3)	−0.035 (18)	0.145 (18)	0.20 (3)

Geometric parameters (Å, º)

O1—C17	1.227 (3)	C11—H11B	0.9600
O2—C22	1.197 (3)	C11—H11C	0.9600
N2—H2	0.8600	C12—H12A	0.9600
N2—C7	1.327 (3)	C12—H12B	0.9600
N2—C9	1.374 (3)	C12—H12C	0.9600
N1—C7	1.338 (2)	C14—H14A	0.9600
N1—C8	1.379 (3)	C14—H14B	0.9600
N1—C10	1.482 (3)	C14—H14C	0.9600

C7—C1	1.480 (3)	C20—H20A	0.9600
C8—H8	0.9300	C20—H20B	0.9600
C8—C9	1.344 (3)	C20—H20C	0.9600
C1—C6	1.400 (3)	C16—H16A	0.9600
C1—C2	1.389 (3)	C16—H16B	0.9600
C6—C17	1.501 (3)	C16—H16C	0.9600
C6—C5	1.388 (3)	C23—C25	1.537 (5)
C9—C13	1.510 (3)	C23—C26	1.530 (5)
N3—C17	1.347 (3)	C23—C24	1.516 (5)
N3—C21	1.451 (3)	C25—H25A	0.9600
N3—C18	1.482 (3)	C25—H25B	0.9600
C10—H10	0.9800	C25—H25C	0.9600
C10—C11	1.515 (4)	C15—H15A	0.9600
C10—C12	1.508 (4)	C15—H15B	0.9600
C2—H2A	0.9300	C15—H15C	0.9600
C2—C3	1.379 (3)	C19—H19A	0.9600
C5—H5	0.9300	C19—H19B	0.9600
C5—C4	1.373 (3)	C19—H19C	0.9600
C4—H4	0.9300	C26—H26A	0.9600
C4—C3	1.376 (4)	C26—H26B	0.9600
C21—H21A	0.9700	C26—H26C	0.9600
C21—H21B	0.9700	C24—H24A	0.9600
C21—C22	1.524 (4)	C24—H24B	0.9600
C13—C14	1.532 (4)	C24—H24C	0.9600
C13—C16	1.532 (4)	Cl1—O3	1.350 (3)
C13—C15	1.524 (4)	Cl1—O4A	1.380 (7)
C3—H3	0.9300	Cl1—O5A	1.333 (6)
C22—C23	1.526 (4)	Cl1—O6A	1.334 (6)
C18—H18	0.9800	Cl1—O6B	1.385 (7)
C18—C20	1.527 (4)	Cl1—O4B	1.306 (8)
C18—C19	1.518 (4)	Cl1—O5B	1.329 (9)
C11—H11A	0.9600		
C7—N2—H2	124.6	C10—C12—H12A	109.5
C7—N2—C9	110.85 (17)	C10—C12—H12B	109.5
C9—N2—H2	124.6	C10—C12—H12C	109.5
C7—N1—C8	108.12 (17)	H12A—C12—H12B	109.5
C7—N1—C10	126.04 (18)	H12A—C12—H12C	109.5
C8—N1—C10	125.83 (17)	H12B—C12—H12C	109.5
N2—C7—N1	107.20 (17)	C13—C14—H14A	109.5
N2—C7—C1	122.99 (17)	C13—C14—H14B	109.5
N1—C7—C1	129.68 (18)	C13—C14—H14C	109.5
N1—C8—H8	125.7	H14A—C14—H14B	109.5
C9—C8—N1	108.64 (18)	H14A—C14—H14C	109.5
C9—C8—H8	125.7	H14B—C14—H14C	109.5
C6—C1—C7	122.16 (18)	C18—C20—H20A	109.5
C2—C1—C7	117.89 (19)	C18—C20—H20B	109.5
C2—C1—C6	119.65 (19)	C18—C20—H20C	109.5

C1—C6—C17	120.04 (18)	H20A—C20—H20B	109.5
C5—C6—C1	119.0 (2)	H20A—C20—H20C	109.5
C5—C6—C17	120.9 (2)	H20B—C20—H20C	109.5
N2—C9—C13	121.92 (19)	C13—C16—H16A	109.5
C8—C9—N2	105.19 (18)	C13—C16—H16B	109.5
C8—C9—C13	132.8 (2)	C13—C16—H16C	109.5
C17—N3—C21	116.5 (2)	H16A—C16—H16B	109.5
C17—N3—C18	124.95 (18)	H16A—C16—H16C	109.5
C21—N3—C18	118.49 (19)	H16B—C16—H16C	109.5
O1—C17—C6	119.5 (2)	C22—C23—C25	112.1 (3)
O1—C17—N3	121.9 (2)	C22—C23—C26	106.6 (3)
N3—C17—C6	118.65 (19)	C26—C23—C25	107.3 (3)
N1—C10—H10	108.4	C24—C23—C22	109.1 (3)
N1—C10—C11	109.6 (2)	C24—C23—C25	113.0 (4)
N1—C10—C12	109.8 (2)	C24—C23—C26	108.5 (4)
C11—C10—H10	108.4	C23—C25—H25A	109.5
C12—C10—H10	108.4	C23—C25—H25B	109.5
C12—C10—C11	112.3 (2)	C23—C25—H25C	109.5
C1—C2—H2A	119.9	H25A—C25—H25B	109.5
C3—C2—C1	120.2 (2)	H25A—C25—H25C	109.5
C3—C2—H2A	119.9	H25B—C25—H25C	109.5
C6—C5—H5	119.6	C13—C15—H15A	109.5
C4—C5—C6	120.8 (2)	C13—C15—H15B	109.5
C4—C5—H5	119.6	C13—C15—H15C	109.5
C5—C4—H4	119.9	H15A—C15—H15B	109.5
C5—C4—C3	120.2 (2)	H15A—C15—H15C	109.5
C3—C4—H4	119.9	H15B—C15—H15C	109.5
N3—C21—H21A	109.2	C18—C19—H19A	109.5
N3—C21—H21B	109.2	C18—C19—H19B	109.5
N3—C21—C22	112.0 (2)	C18—C19—H19C	109.5
H21A—C21—H21B	107.9	H19A—C19—H19B	109.5
C22—C21—H21A	109.2	H19A—C19—H19C	109.5
C22—C21—H21B	109.2	H19B—C19—H19C	109.5
C9—C13—C14	108.0 (2)	C23—C26—H26A	109.5
C9—C13—C16	109.2 (2)	C23—C26—H26B	109.5
C9—C13—C15	108.9 (2)	C23—C26—H26C	109.5
C14—C13—C16	110.0 (3)	H26A—C26—H26B	109.5
C15—C13—C14	110.6 (3)	H26A—C26—H26C	109.5
C15—C13—C16	110.1 (3)	H26B—C26—H26C	109.5
C2—C3—H3	119.9	C23—C24—H24A	109.5
C4—C3—C2	120.2 (2)	C23—C24—H24B	109.5
C4—C3—H3	119.9	C23—C24—H24C	109.5
O2—C22—C21	120.6 (2)	H24A—C24—H24B	109.5
O2—C22—C23	121.1 (3)	H24A—C24—H24C	109.5
C21—C22—C23	118.3 (2)	H24B—C24—H24C	109.5
N3—C18—H18	107.6	O3—Cl1—O4A	103.6 (6)
N3—C18—C20	110.1 (2)	O3—Cl1—O6B	100.5 (6)
N3—C18—C19	111.7 (2)	O5A—Cl1—O3	117.5 (5)

C20—C18—H18	107.6	O5A—Cl1—O4A	105.7 (6)
C19—C18—H18	107.6	O5A—Cl1—O6A	110.3 (6)
C19—C18—C20	112.1 (2)	O6A—Cl1—O3	110.4 (5)
C10—C11—H11A	109.5	O6A—Cl1—O4A	108.7 (7)
C10—C11—H11B	109.5	O4B—Cl1—O3	115.8 (7)
C10—C11—H11C	109.5	O4B—Cl1—O6B	108.4 (8)
H11A—C11—H11B	109.5	O4B—Cl1—O5B	111.5 (8)
H11A—C11—H11C	109.5	O5B—Cl1—O3	111.3 (8)
H11B—C11—H11C	109.5	O5B—Cl1—O6B	108.6 (9)
O2—C22—C23—C25	148.6 (4)	C1—C2—C3—C4	0.5 (4)
O2—C22—C23—C26	−94.3 (4)	C6—C1—C2—C3	0.5 (4)
O2—C22—C23—C24	22.6 (5)	C6—C5—C4—C3	−0.4 (4)
N2—C7—C1—C6	103.3 (2)	C9—N2—C7—N1	0.5 (2)
N2—C7—C1—C2	−70.4 (3)	C9—N2—C7—C1	176.64 (19)
N2—C9—C13—C14	−56.9 (3)	N3—C21—C22—O2	8.0 (4)
N2—C9—C13—C16	62.6 (3)	N3—C21—C22—C23	−172.3 (2)
N2—C9—C13—C15	−177.1 (3)	C17—C6—C5—C4	178.5 (2)
N1—C7—C1—C6	−81.5 (3)	C17—N3—C21—C22	−78.2 (3)
N1—C7—C1—C2	104.8 (3)	C17—N3—C18—C20	−102.9 (3)
N1—C8—C9—N2	0.8 (2)	C17—N3—C18—C19	131.9 (2)
N1—C8—C9—C13	−175.9 (2)	C10—N1—C7—N2	178.70 (19)
C7—N2—C9—C8	−0.8 (2)	C10—N1—C7—C1	2.9 (3)
C7—N2—C9—C13	176.3 (2)	C10—N1—C8—C9	−179.2 (2)
C7—N1—C8—C9	−0.5 (2)	C2—C1—C6—C17	−178.5 (2)
C7—N1—C10—C11	133.0 (2)	C2—C1—C6—C5	−1.5 (3)
C7—N1—C10—C12	−103.2 (3)	C5—C6—C17—O1	−98.6 (3)
C7—C1—C6—C17	7.9 (3)	C5—C6—C17—N3	81.1 (3)
C7—C1—C6—C5	−175.1 (2)	C5—C4—C3—C2	−0.6 (4)
C7—C1—C2—C3	174.4 (2)	C21—N3—C17—O1	−7.9 (3)
C8—N1—C7—N2	0.0 (2)	C21—N3—C17—C6	172.35 (19)
C8—N1—C7—C1	−175.8 (2)	C21—N3—C18—C20	79.4 (3)
C8—N1—C10—C11	−48.5 (3)	C21—N3—C18—C19	−45.8 (3)
C8—N1—C10—C12	75.3 (3)	C21—C22—C23—C25	−31.2 (4)
C8—C9—C13—C14	119.3 (3)	C21—C22—C23—C26	85.9 (4)
C8—C9—C13—C16	−121.2 (3)	C21—C22—C23—C24	−157.1 (4)
C8—C9—C13—C15	−0.9 (4)	C18—N3—C17—O1	174.4 (2)
C1—C6—C17—O1	78.3 (3)	C18—N3—C17—C6	−5.4 (3)
C1—C6—C17—N3	−101.9 (2)	C18—N3—C21—C22	99.7 (3)
C1—C6—C5—C4	1.5 (4)		

Hydrogen-bond geometry (Å, º)

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O3	0.86	1.94	2.752 (4)	157
C2—H2A···O1[i]	0.93	2.44	3.319 (3)	158
C5—H5···O5A[ii]	0.93	2.55	3.328 (11)	141

C8—H8···O4*A*[iii]	0.93	2.36	3.285 (8)	173
C10—H10···O1	0.98	2.55	3.167 (3)	121

Symmetry codes: (i) −*x*+3/2, *y*+1/2, −*z*+3/2; (ii) −*x*+1/2, *y*−1/2, −*z*+3/2; (iii) *x*+1, *y*, *z*.