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Crystal structure of bis(1-benzyl-1*H*-1,2,4-triazole) perchloric acid monosolvate

Yong-Qi Qin,[a]* Jin-hui Xue,[b] Yuan-Biao Qiao[a] and Zi-Feng Zhang[b]

[a]Laboratory of Medicinal Chemistry, Lvliang University, Lvliang, Shanxi 033001, People's Republic of China, and [b]Department of Chemistry and Chemical Engineering, Lvliang University, Lvliang, Shanxi 033001, People's Republic of China. *Correspondence e-mail: qinyq2003@163.com

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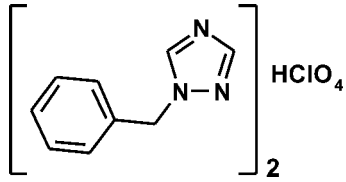
The title compound, $2C_9H_9N_3\cdot HClO_4$, was prepared by reaction of 1-benzyl-1*H*-1,2,4-triazole and $HClO_4$ in ethanol at room temperature. The asymmetric unit consists of two molecules of 1-benzyl-1*H*-1,2,4-triazole and one of $HClO_4$ molecule. The benzene and triazole rings make dihedral angles of 85.45 (8) and 84.76 (8)° in the two molecules. The H-atom position of the perchloric acid molecule is split over two O atoms (real peaks on difference map), with site-occupation factors of 0.5. These H atoms form two classical hydrogen bonds [2.546 (5) and 2.620 (4) Å] with the same N atoms in both molecules. Five intermolecular non-classical C—H···O interactions, with C···O distances in the range 3.147 (5)–3.483 (5) Å, are found in the crystal structure.

Keywords: crystal structure; 1*H*-1,2,4-triazole; perchloric acid; antiviral activity.

CCDC reference: 1033730

1. Related literature

For the antiviral activity of triazole derivatives, see: Madan & Taneja (1991); Borisova *et al.* (2007) and of polyligand complexes with metals, see: Xu *et al.* (2004). For a related structure, see: Ji *et al.* (2002).



2. Experimental

2.1. Crystal data

$2C_9H_9N_3\cdot HClO_4$
M_r = 418.84
Monoclinic, $P2_1$
a = 5.7173 (10) Å
b = 7.7671 (12) Å
c = 21.955 (4) Å
β = 95.136 (4)°
V = 971.0 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.24 mm^{-1}
T = 296 K
0.25 × 0.23 × 0.20 mm

2.2. Data collection

Bruker SMART CCD diffractometer
9373 measured reflections
3981 independent reflections
2680 reflections with $I > 2\sigma(I)$
R_{int} = 0.050

2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.137
S = 1.05
3981 reflections
263 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 e Å^{-3}
Absolute structure: Flack (1983), 873 Friedel pairs
Absolute structure parameter: 0.27 (9)

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3A···N6^{i}	0.82	2.04	2.620 (4)	127
O1—H1···N3^{ii}	0.82	1.78	2.546 (5)	154
C10—H10B···O4	0.97	2.35	3.282 (5)	160
C9—H9···O2^{iii}	0.93	2.52	3.352 (6)	150
C1—H1A···O2^{iv}	0.97	2.56	3.483 (5)	158
C17—H17···O4^{v}	0.93	2.43	3.147 (5)	134
C18—H18···O3^{vi}	0.93	2.44	3.185 (5)	137

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); 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*.

Acknowledgements

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Supporting information for this paper is available from the IUCr electronic archives (Reference: RK2425).

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supporting information

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Crystal structure of bis(1-benzyl-1*H*-1,2,4-triazole) perchloric acid monosolvate

Yong-Qi Qin, Jin-hui Xue, Yuan-Biao Qiao and Zi-Feng Zhang

S1. Comment

It is well known, that triazole derivatives possess anti-viral activities (Madan & Taneja, 1991; Borisova *et al.*, 2007). A materials about anti-viral activities of the such polyligand complexes with metals were published Xu *et al.*, 2004. These facts were of a reason for structural study of 1-benzyl-1*H*-1,2,4-triazole $HClO_4$ solvate.

In the molecule of the title compound (Fig. 1), bond lengths and angles are generally normal in benzene and 1,2,4-triazole ring (Ji *et al.*, 2002). The torsion angles of C2—C1—N1—C8 and N1—C1—C2—C3 are -108.2 (4)° and 60.3 (5)°, respectively; C11—C10—N4—C17 and N4—C10—C11—C12 are 115.2 (4)° and 124.3 (4)° respectively. The dihedral angle formed by the benzene and the triazole ring is 85.45 (8)° and 84.76 (8)° for first and second molecules respectively.

There are some classical O—H···N and non-classical C—H···O intermolecular interactions stabilize the title crystal structure (Fig. 2).

S2. Experimental

The title compound was prepared by reaction of benzyl chloride (0.05 mol), triazole (0.05 mol), potassium carbonate (0.06 mol) and potassium iodide (0.5 g) in the acetone solution (40 ml) at 333 K for 8 h, filtering, evaporating the solvent, affording the tile compound (6.2 g, yield 78%) by solidification in the etanol solution of $HClO_4$ (5%, 15 ml). In the reaction, potassium carbonate can powerfully adsorb HCl to promote the reaction and potassium iodide is catalyst. Single crystals of the title compound suitable for X-ray measurements was obtained by recrystallization from ethanol/acetone (*v*/*v* = 1:1) at room temperature.

S3. Refinement

The H atoms were fixed geometrically and allowed to ride on their attached atoms, with C—H distances = 0.93–0.97 Å; O—H = 0.82 Å and U_{iso}(H) = 1.2–1.5U_{eq}(C, O).

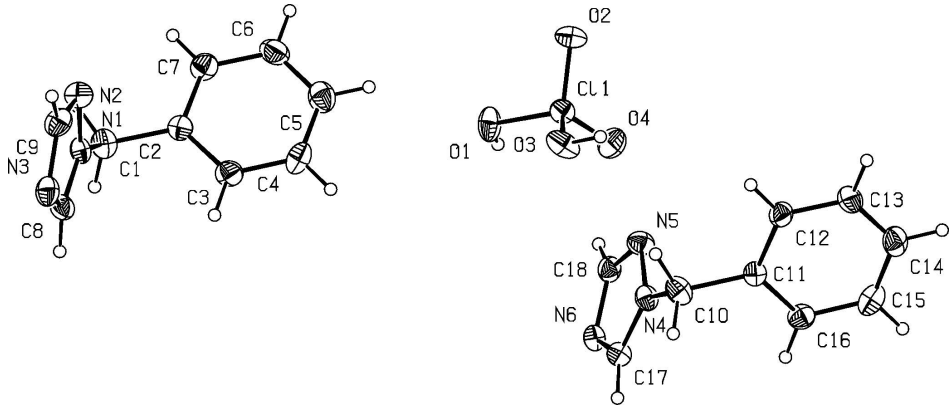

Figure 1

The molecular structure of the title compound with the atom numbering scheme. The displacement ellipsoids are drawn at the 40% probability level H atoms are presented as a small spheres of arbitrary radius.

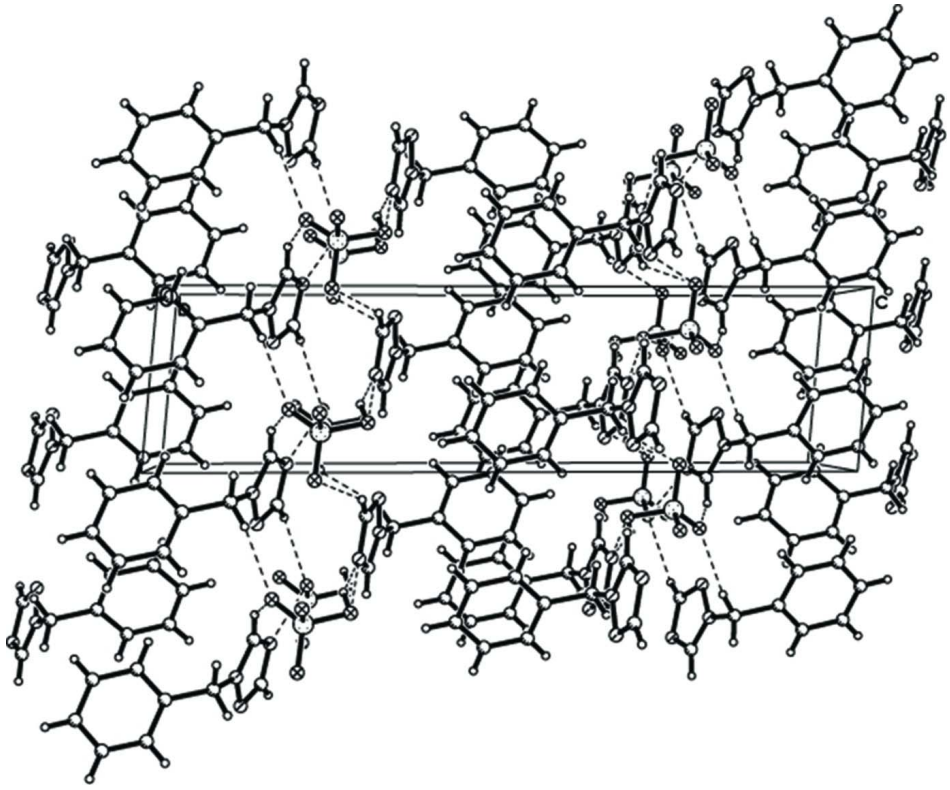

Figure 2

The packing of the title compound, viewed down the *b* axis, showing short contact (dashed lines).

Bis(1-benzyl-1*H*-1,2,4-triazole) perchloric acid monosolvate

Crystal data

$2C_9H_9N_3{\cdot}HClO_4$
M_r = 418.84
Monoclinic, $P2_1$
a = 5.7173 (10) Å
b = 7.7671 (12) Å
c = 21.955 (4) Å
β = 95.136 (4)°
V = 971.0 (3) Å^3

$Z = 2$
$F(000) = 436$
$D_x = 1.433$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 637 reflections
$\theta = 3.2–19.6°$
$\mu = 0.24$ mm^{-1}
$T = 296$ K
Rectangle, colourless
0.25 × 0.23 × 0.20 mm

Data collection

Bruker SMART CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
9373 measured reflections
3981 independent reflections
2680 reflections with $I > 2\sigma(I)$
$R_{int} = 0.050$
$\theta_{max} = 28.1°$, $\theta_{min} = 2.8°$
$h = -7 \rightarrow 7$
$k = -9 \rightarrow 9$
$l = -28 \rightarrow 28$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.053$
$wR(F^2) = 0.137$
$S = 1.05$
3981 reflections
263 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0604P)^2 + 0.021P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.35$ e Å^{-3}
$\Delta\rho_{min} = -0.39$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.007 (2)
Absolute structure: Flack (1983) parameter determined using 873 quotients
Absolute structure parameter: 0.27 (9)

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'s 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	0.22466 (15)	0.25879 (13)	0.75737 (4)	0.0376 (3)	
O2	−0.0268 (4)	0.2501 (5)	0.75956 (13)	0.0501 (7)	
O3	0.3257 (5)	0.0851 (3)	0.75971 (14)	0.0506 (8)	
H3A	0.2975	0.0380	0.7917	0.076*	0.50
O1	0.2712 (5)	0.3307 (4)	0.69478 (12)	0.0520 (8)	
H1	0.3440	0.4193	0.7039	0.078*	0.50
O4	0.3397 (5)	0.3708 (4)	0.80363 (14)	0.0579 (9)	
N2	0.1586 (5)	0.2466 (5)	0.33197 (15)	0.0446 (8)	
C5	0.1887 (8)	0.5483 (7)	0.5465 (2)	0.0544 (12)	
H5	0.1552	0.5518	0.5871	0.065*	
N3	0.4745 (6)	0.0982 (5)	0.31116 (16)	0.0459 (9)	
C9	0.2415 (8)	0.0996 (6)	0.3156 (2)	0.0474 (11)	
H9	0.1473	0.0032	0.3076	0.057*	

N1	0.3519 (6)	0.3489 (4)	0.33810 (14)	0.0351 (8)
C1	0.3406 (8)	0.5273 (5)	0.35882 (18)	0.0443 (11)
H1A	0.2189	0.5877	0.3336	0.053*
H1B	0.4891	0.5838	0.3539	0.053*
C6	0.0396 (8)	0.6210 (7)	0.5020 (2)	0.0549 (13)
H6	−0.0967	0.6744	0.5125	0.066*
C2	0.2893 (7)	0.5377 (5)	0.42460 (18)	0.0364 (9)
C8	0.5381 (6)	0.2598 (7)	0.32578 (17)	0.0417 (9)
H8	0.6903	0.3026	0.3271	0.050*
C4	0.3899 (8)	0.4693 (6)	0.53045 (19)	0.0507 (12)
H4	0.4927	0.4191	0.5605	0.061*
C7	0.0878 (7)	0.6168 (6)	0.4414 (2)	0.0460 (11)
H7	−0.0161	0.6675	0.4117	0.055*
C3	0.4401 (7)	0.4640 (6)	0.4706 (2)	0.0454 (11)
H3	0.5770	0.4104	0.4606	0.054*
N5	0.7031 (5)	0.7708 (5)	0.83783 (15)	0.0417 (8)
N4	0.8811 (6)	0.6541 (4)	0.84658 (14)	0.0366 (8)
C18	0.7984 (7)	0.9014 (6)	0.81290 (17)	0.0395 (10)
H18	0.7188	1.0027	0.8019	0.047*
C16	0.9431 (7)	0.5756 (6)	0.98327 (19)	0.0420 (10)
H16	1.0821	0.6247	0.9726	0.050*
N6	1.0286 (6)	0.8733 (4)	0.80462 (14)	0.0356 (8)
C11	0.7924 (6)	0.4980 (5)	0.93922 (17)	0.0317 (9)
C12	0.5874 (7)	0.4219 (6)	0.95742 (18)	0.0405 (10)
H12	0.4834	0.3681	0.9284	0.049*
C10	0.8470 (8)	0.4849 (5)	0.87376 (19)	0.0441 (11)
H10A	0.9882	0.4167	0.8716	0.053*
H10B	0.7192	0.4259	0.8503	0.053*
C14	0.6861 (8)	0.5066 (6)	1.0598 (2)	0.0485 (12)
H14	0.6493	0.5113	1.1002	0.058*
C17	1.0749 (7)	0.7164 (5)	0.82694 (18)	0.0357 (10)
H17	1.2192	0.6605	0.8284	0.043*
C15	0.8882 (8)	0.5809 (6)	1.0437 (2)	0.0507 (12)
H15	0.9894	0.6352	1.0732	0.061*
C13	0.5389 (8)	0.4258 (6)	1.01696 (19)	0.0482 (12)
H13	0.4038	0.3727	1.0284	0.058*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0384 (5)	0.0346 (5)	0.0404 (5)	0.0025 (5)	0.0060 (4)	0.0025 (5)
O2	0.0300 (13)	0.0547 (19)	0.0666 (19)	0.0054 (16)	0.0088 (12)	−0.0001 (19)
O3	0.0517 (17)	0.0285 (16)	0.075 (2)	0.0139 (14)	0.0271 (15)	0.0174 (15)
O1	0.078 (2)	0.0441 (18)	0.0338 (16)	−0.0108 (16)	0.0065 (15)	0.0126 (13)
O4	0.0575 (19)	0.065 (2)	0.0497 (19)	−0.0129 (17)	−0.0052 (15)	−0.0157 (17)
N2	0.0429 (17)	0.039 (2)	0.052 (2)	0.000 (2)	0.0037 (15)	−0.003 (2)
C5	0.063 (3)	0.053 (3)	0.048 (3)	−0.005 (3)	0.010 (2)	−0.010 (2)
N3	0.057 (2)	0.045 (2)	0.035 (2)	−0.0044 (19)	0.0028 (17)	−0.0077 (17)

C9	0.050 (3)	0.044 (3)	0.047 (3)	−0.010 (2)	−0.005 (2)	−0.008 (2)
N1	0.0440 (19)	0.033 (2)	0.0289 (17)	0.0003 (16)	0.0082 (15)	−0.0037 (15)
C1	0.057 (3)	0.031 (3)	0.045 (3)	−0.001 (2)	0.007 (2)	0.007 (2)
C6	0.042 (3)	0.066 (4)	0.059 (3)	0.001 (2)	0.014 (2)	−0.014 (3)
C2	0.040 (2)	0.029 (2)	0.040 (2)	−0.0019 (18)	0.0032 (18)	−0.0044 (19)
C8	0.041 (2)	0.045 (3)	0.040 (2)	−0.009 (3)	0.0093 (17)	−0.002 (3)
C4	0.065 (3)	0.046 (3)	0.039 (3)	0.003 (2)	−0.011 (2)	−0.003 (2)
C7	0.048 (3)	0.041 (3)	0.048 (3)	0.008 (2)	0.001 (2)	−0.001 (2)
C3	0.043 (2)	0.043 (3)	0.050 (3)	0.009 (2)	0.004 (2)	−0.010 (2)
N5	0.0370 (16)	0.040 (2)	0.049 (2)	0.0052 (18)	0.0065 (14)	0.003 (2)
N4	0.042 (2)	0.033 (2)	0.0354 (18)	−0.0029 (15)	0.0076 (16)	0.0000 (16)
C18	0.044 (2)	0.040 (3)	0.034 (2)	0.007 (2)	0.0028 (18)	0.005 (2)
C16	0.040 (2)	0.039 (2)	0.047 (3)	−0.0060 (19)	0.0015 (19)	0.000 (2)
N6	0.0432 (19)	0.033 (2)	0.0307 (18)	0.0002 (16)	0.0060 (15)	−0.0007 (16)
C11	0.039 (2)	0.022 (2)	0.034 (2)	0.0028 (17)	0.0034 (17)	0.0023 (17)
C12	0.040 (2)	0.045 (3)	0.036 (2)	−0.0062 (19)	0.0009 (18)	0.007 (2)
C10	0.053 (3)	0.033 (2)	0.049 (3)	−0.002 (2)	0.016 (2)	0.008 (2)
C14	0.060 (3)	0.047 (3)	0.040 (2)	0.014 (2)	0.008 (2)	0.014 (2)
C17	0.037 (2)	0.031 (3)	0.039 (2)	−0.0017 (18)	0.0049 (17)	0.0010 (17)
C15	0.062 (3)	0.043 (3)	0.044 (3)	−0.001 (2)	−0.012 (2)	0.002 (2)
C13	0.046 (3)	0.058 (3)	0.043 (3)	−0.005 (2)	0.012 (2)	0.013 (2)

Geometric parameters (Å, º)

Cl1—O2	1.444 (2)	C4—H4	0.9300
Cl1—O4	1.449 (3)	C7—H7	0.9300
Cl1—O3	1.466 (3)	C3—H3	0.9300
Cl1—O1	1.529 (3)	N5—C18	1.295 (5)
O3—H3A	0.8200	N5—N4	1.363 (4)
O1—H1	0.8200	N4—C17	1.317 (5)
N2—C9	1.299 (6)	N4—C10	1.464 (5)
N2—N1	1.358 (4)	C18—N6	1.362 (5)
C5—C6	1.359 (7)	C18—H18	0.9300
C5—C4	1.377 (6)	C16—C11	1.375 (5)
C5—H5	0.9300	C16—C15	1.390 (6)
N3—C8	1.338 (6)	C16—H16	0.9300
N3—C9	1.345 (5)	N6—C17	1.331 (5)
C9—H9	0.9300	C11—C12	1.402 (5)
N1—C8	1.318 (5)	C11—C10	1.501 (5)
N1—C1	1.462 (5)	C12—C13	1.361 (5)
C1—C2	1.501 (5)	C12—H12	0.9300
C1—H1A	0.9700	C10—H10A	0.9700
C1—H1B	0.9700	C10—H10B	0.9700
C6—C7	1.384 (6)	C14—C13	1.359 (6)
C6—H6	0.9300	C14—C15	1.367 (6)
C2—C7	1.384 (5)	C14—H14	0.9300
C2—C3	1.391 (6)	C17—H17	0.9300
C8—H8	0.9300	C15—H15	0.9300

C4—C3	1.370 (6)	C13—H13	0.9300
O2—Cl1—O4	113.29 (19)	C2—C7—H7	119.7
O2—Cl1—O3	110.2 (2)	C4—C3—C2	121.0 (4)
O4—Cl1—O3	112.0 (2)	C4—C3—H3	119.5
O2—Cl1—O1	107.50 (18)	C2—C3—H3	119.5
O4—Cl1—O1	107.82 (19)	C18—N5—N4	104.1 (3)
O3—Cl1—O1	105.54 (17)	C17—N4—N5	110.4 (3)
Cl1—O3—H3A	109.5	C17—N4—C10	127.6 (3)
Cl1—O1—H1	102.2	N5—N4—C10	122.0 (3)
C9—N2—N1	103.2 (3)	N5—C18—N6	112.3 (4)
C6—C5—C4	119.1 (4)	N5—C18—H18	123.9
C6—C5—H5	120.4	N6—C18—H18	123.9
C4—C5—H5	120.4	C11—C16—C15	120.2 (4)
C8—N3—C9	103.0 (4)	C11—C16—H16	119.9
N2—C9—N3	114.6 (4)	C15—C16—H16	119.9
N2—C9—H9	122.7	C17—N6—C18	105.1 (4)
N3—C9—H9	122.7	C16—C11—C12	118.1 (4)
C8—N1—N2	109.7 (3)	C16—C11—C10	122.2 (4)
C8—N1—C1	128.4 (4)	C12—C11—C10	119.7 (4)
N2—N1—C1	121.8 (3)	C13—C12—C11	120.8 (4)
N1—C1—C2	111.6 (3)	C13—C12—H12	119.6
N1—C1—H1A	109.3	C11—C12—H12	119.6
C2—C1—H1A	109.3	N4—C10—C11	112.1 (3)
N1—C1—H1B	109.3	N4—C10—H10A	109.2
C2—C1—H1B	109.3	C11—C10—H10A	109.2
H1A—C1—H1B	108.0	N4—C10—H10B	109.2
C5—C6—C7	120.9 (4)	C11—C10—H10B	109.2
C5—C6—H6	119.5	H10A—C10—H10B	107.9
C7—C6—H6	119.5	C13—C14—C15	120.1 (4)
C7—C2—C3	117.7 (4)	C13—C14—H14	120.0
C7—C2—C1	121.3 (4)	C15—C14—H14	120.0
C3—C2—C1	121.0 (4)	N4—C17—N6	108.1 (3)
N1—C8—N3	109.6 (3)	N4—C17—H17	125.9
N1—C8—H8	125.2	N6—C17—H17	125.9
N3—C8—H8	125.2	C14—C15—C16	120.2 (4)
C3—C4—C5	120.6 (4)	C14—C15—H15	119.9
C3—C4—H4	119.7	C16—C15—H15	119.9
C5—C4—H4	119.7	C14—C13—C12	120.6 (4)
C6—C7—C2	120.6 (4)	C14—C13—H13	119.7
C6—C7—H7	119.7	C12—C13—H13	119.7
N1—N2—C9—N3	0.6 (5)	C18—N5—N4—C17	−0.1 (4)
C8—N3—C9—N2	−0.5 (5)	C18—N5—N4—C10	−179.5 (3)
C9—N2—N1—C8	−0.4 (4)	N4—N5—C18—N6	0.7 (4)
C9—N2—N1—C1	−177.4 (4)	N5—C18—N6—C17	−1.0 (4)
C8—N1—C1—C2	−108.2 (4)	C15—C16—C11—C12	−1.5 (6)
N2—N1—C1—C2	68.1 (5)	C15—C16—C11—C10	−178.3 (4)

C4—C5—C6—C7	−0.1 (8)	C16—C11—C12—C13	0.4 (6)
N1—C1—C2—C7	−118.1 (4)	C10—C11—C12—C13	177.2 (4)
N1—C1—C2—C3	60.3 (5)	C17—N4—C10—C11	115.2 (4)
N2—N1—C8—N3	0.2 (4)	N5—N4—C10—C11	−65.5 (5)
C1—N1—C8—N3	176.9 (4)	C16—C11—C10—N4	−58.9 (5)
C9—N3—C8—N1	0.2 (5)	C12—C11—C10—N4	124.3 (4)
C6—C5—C4—C3	0.1 (8)	N5—N4—C17—N6	−0.5 (4)
C5—C6—C7—C2	0.2 (7)	C10—N4—C17—N6	178.9 (4)
C3—C2—C7—C6	−0.2 (6)	C18—N6—C17—N4	0.8 (4)
C1—C2—C7—C6	178.2 (4)	C13—C14—C15—C16	0.6 (7)
C5—C4—C3—C2	−0.2 (7)	C11—C16—C15—C14	1.0 (6)
C7—C2—C3—C4	0.2 (6)	C15—C14—C13—C12	−1.8 (7)
C1—C2—C3—C4	−178.2 (4)	C11—C12—C13—C14	1.3 (6)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3*A*···N6^{i}	0.82	2.04	2.620 (4)	127
O1—H1···N3^{ii}	0.82	1.78	2.546 (5)	154
C10—H10*B*···O4	0.97	2.35	3.282 (5)	160
C9—H9···O2^{iii}	0.93	2.52	3.352 (6)	150
C1—H1*A*···O2^{iv}	0.97	2.56	3.483 (5)	158
C17—H17···O4^{v}	0.93	2.43	3.147 (5)	134
C18—H18···O3^{vi}	0.93	2.44	3.185 (5)	137

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