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Bis(creatininium) 3-nitrophthalate monohydrate

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Keywords: crystal structure; creatininium; phthalate; glomerular filtration rate; hydrogen bonding.

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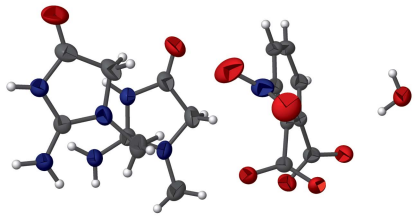
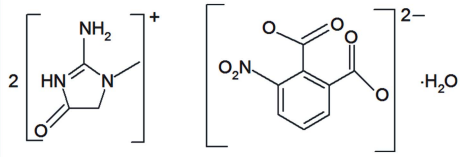
Structural data: full structural data are available from iucrdata.iucr.org

In the title hydrated molecular salt, $2C_4H_8N_3O^+\cdot C_8H_3NO_6^{2-}\cdot H_2O$, the dihedral angles between the benzene ring and the nitro group and the carboxylate groups are 48.0 (2), 55.3 (2) and 60.7 (2)°, respectively. In the crystal, the components are linked by N—H···O, O—H···O and C—H···O hydrogen bonds, generating a two-dimensional network parallel to (102).

3D view



Chemical scheme



Structure description

Creatinine (systematic name: 2-imino-1-methylimidazolidin-4-one) and its derivatives display a range of biological activity. In particular, creatinine is an indicator of renal function. In understanding renal dysfunction, the determination of creatinine is more important than that of urea (Sharma *et al.*, 2004). Creatinine clearance is used to determine the glomerular filtration rate (GFR) of the kidneys (Mădăraş & Buck, 1996) and various disease states in biological fluids can be indicated by an abnormal level of creatinine (Narayanan & Appleton, 1980). We report here the structure of the protonated creatinine derivative bis-creatininium 3-nitrophthalate that crystallizes as a monohydrate.

The asymmetric unit of the title compound comprises two protonated creatinine cations, one doubly deprotonated 3-nitrophthalic acid anion and a water molecule of crystallization (Fig. 1). The geometric parameters of the title molecule agree well with those reported for similar similar structures (Jahubar Ali *et al.*, 2011, 2012). The packing features N—H···O, O—H···O and C—H···O hydrogen bonds, which generate a two-dimensional network parallel to (102) (Table 1, Fig. 2).

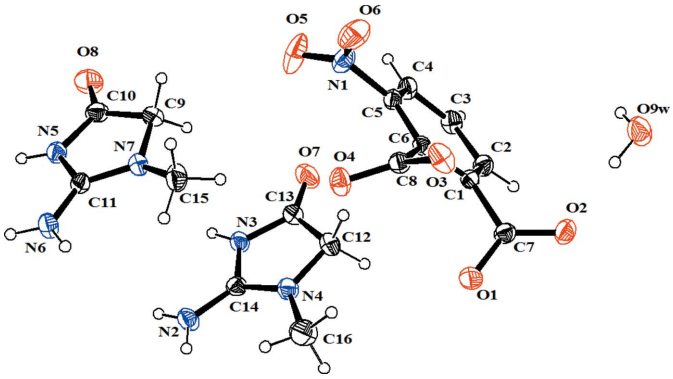


Figure 1
The molecular structure with atom labels and 30% probability displacement ellipsoids for non-H atoms.

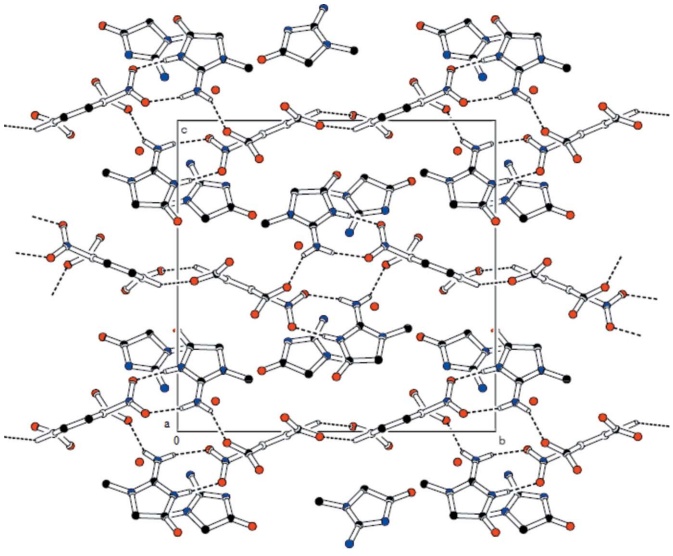


Figure 2
The packing, viewed down the *a* axis. Hydrogen bonds are shown as dashed lines.

Synthesis and crystallization

Creatinine and 3-nitrophthalic acid in 2:1 molar ratio were dissolved in deionized water. The solution was stirred well, filtered and kept in a dust-free environment. Crystals were obtained from the mother solution after 10 d (yield 95%).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

References

Bruker (2008). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.

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

D—H···A	D—H	H···A	D···A	D—H···A
O9W—H9WA···O2	0.86 (1)	1.94 (2)	2.7856 (18)	168 (2)
O9W—H9WB···O8^{i}	0.85 (1)	2.16 (2)	2.9241 (18)	149 (2)
N2—H2A···O3^{ii}	0.86	2.00	2.7899 (17)	152
N2—H2B···O2^{iii}	0.86	1.95	2.8000 (17)	168
N3—H3A···O1^{iii}	0.86	1.77	2.6275 (15)	177
N5—H5···O4^{iv}	0.86	1.84	2.6836 (16)	166
N6—H6A···O9W^{v}	0.86	1.96	2.7952 (17)	163
N6—H6B···O3^{iv}	0.86	1.94	2.7900 (16)	171
C4—H4···O5^{i}	0.93	2.59	3.2071 (19)	124
C9—H9B···O6^{vi}	0.97	2.47	3.212 (2)	133

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$2C_4H_8N_3O^+\cdot C_8H_3NO_6^{2-}\cdot H_2O$
M_r	455.40
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	295
a, b, c (Å)	7.6682 (3), 16.5504 (6), 16.2358 (7)
β (°)	93.775 (1)
V (Å^3)	2056.04 (14)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.12
Crystal size (mm)	0.30 × 0.25 × 0.20
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Sheldrick, 1996)
T_{min}, T_{max}	0.964, 0.975
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	30566, 3620, 3202
R_{int}	0.023
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.595
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.034, 0.097, 1.04
No. of reflections	3620
No. of parameters	299
No. of restraints	3
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.23, −0.19

Computer programs: *APEX2* and *SAINT* (Bruker, 2008), *SHELXS97* and *SHELXL97* (Sheldrick, 2008) and *PLATON* (Spek, 2009).

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full crystallographic data

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Bis(creatininium) 3-nitrophthalate monohydrate

V. Thayanithi, P. Praveen Kumar and B. Gunasekaran

Bis(2-amino-1-methyl-4-oxo-1*H*-imidazol-3-ium) 3-nitrobenzene-1,2-dioate monohydrate

Crystal data

$2C_4H_8N_3O^+\cdot C_8H_3NO_6^{2-}\cdot H_2O$
M_r = 455.40
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 7.6682 (3) Å
b = 16.5504 (6) Å
c = 16.2358 (7) Å
β = 93.775 (1)°
V = 2056.04 (14) Å^3
Z = 4
$F(000)$ = 952
D_x = 1.471 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3032 reflections
θ = 2.5–25.0°
μ = 0.12 mm^{-1}
T = 295 K
Block, colourless
0.30 × 0.25 × 0.20 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 0 pixels mm^{-1}
ω and φ scans
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
T_{min} = 0.964, T_{max} = 0.975
30566 measured reflections
3620 independent reflections
3202 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 25.0°, θ_{min} = 2.5°
h = −9→9
k = −19→19
l = −19→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.097
S = 1.04
3620 reflections
299 parameters
3 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
$w = 1/[\sigma^2(F_o^2) + (0.0511P)^2 + 0.6212P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O4	0.31739 (13)	0.24338 (6)	0.37689 (7)	0.0426 (3)
O2	−0.20496 (15)	0.39851 (6)	0.44152 (7)	0.0468 (3)

O1	−0.05094 (16)	0.36012 (6)	0.33692 (7)	0.0500 (3)
O7	−0.12906 (18)	−0.00022 (8)	0.32383 (8)	0.0623 (4)
O3	0.26695 (14)	0.34371 (6)	0.46389 (7)	0.0455 (3)
O8	0.37908 (18)	−0.23485 (8)	0.30455 (8)	0.0650 (4)
N4	0.04747 (17)	0.14441 (7)	0.19650 (8)	0.0411 (3)
N5	0.50199 (16)	−0.15212 (7)	0.21091 (8)	0.0382 (3)
H5	0.5431	−0.1882	0.1794	0.046*
C1	−0.09432 (17)	0.26573 (8)	0.44182 (8)	0.0292 (3)
C5	0.08351 (17)	0.15554 (8)	0.48841 (8)	0.0306 (3)
O6	0.36494 (17)	0.16305 (9)	0.54522 (9)	0.0698 (4)
N1	0.25658 (17)	0.12099 (8)	0.50719 (9)	0.0455 (3)
N7	0.43615 (16)	−0.03075 (8)	0.25712 (7)	0.0392 (3)
N2	0.15811 (18)	0.06240 (8)	0.09368 (8)	0.0446 (3)
H2A	0.1982	0.1028	0.0675	0.054*
H2B	0.1711	0.0141	0.0755	0.054*
C6	0.07245 (17)	0.23258 (7)	0.45540 (7)	0.0275 (3)
N6	0.59974 (16)	−0.04045 (7)	0.13985 (8)	0.0406 (3)
H6A	0.6065	0.0111	0.1343	0.049*
H6B	0.6479	−0.0718	0.1057	0.049*
N3	0.01716 (15)	0.01224 (7)	0.20550 (7)	0.0367 (3)
H3A	0.0275	−0.0380	0.1932	0.044*
O5	0.28472 (18)	0.05264 (8)	0.48399 (11)	0.0811 (5)
C2	−0.24056 (18)	0.22093 (9)	0.45977 (9)	0.0357 (3)
H2	−0.3512	0.2436	0.4513	0.043*
C14	0.07773 (18)	0.07435 (8)	0.16086 (8)	0.0341 (3)
C4	−0.05969 (19)	0.11000 (8)	0.50609 (9)	0.0364 (3)
H4	−0.0464	0.0584	0.5282	0.044*
C8	0.23328 (17)	0.27727 (8)	0.43044 (8)	0.0314 (3)
C3	−0.22333 (19)	0.14322 (9)	0.49004 (9)	0.0387 (3)
H3	−0.3224	0.1132	0.4997	0.046*
C7	−0.11757 (18)	0.34859 (8)	0.40421 (9)	0.0338 (3)
C9	0.3674 (2)	−0.08763 (10)	0.31486 (9)	0.0468 (4)
H9A	0.2420	−0.0815	0.3172	0.056*
H9B	0.4229	−0.0807	0.3698	0.056*
C11	0.51691 (17)	−0.07093 (8)	0.19967 (8)	0.0333 (3)
C10	0.4126 (2)	−0.16844 (10)	0.27923 (10)	0.0445 (4)
C13	−0.0626 (2)	0.04049 (10)	0.27279 (9)	0.0423 (4)
C15	0.4564 (2)	0.05471 (10)	0.27549 (11)	0.0492 (4)
H15A	0.5508	0.0621	0.3166	0.074*
H15B	0.3502	0.0752	0.2958	0.074*
H15C	0.4814	0.0833	0.2262	0.074*
C12	−0.0482 (2)	0.13135 (10)	0.26946 (10)	0.0480 (4)
H12A	−0.1627	0.1564	0.2638	0.058*
H12B	0.0155	0.1524	0.3185	0.058*
C16	0.0946 (3)	0.22366 (10)	0.16828 (11)	0.0602 (5)
H16A	0.1949	0.2195	0.1361	0.090*
H16B	0.1217	0.2580	0.2150	0.090*
H16C	−0.0013	0.2462	0.1349	0.090*

O9W	−0.3299 (2)	0.38052 (7)	0.59774 (8)	0.0656 (4)
H9WA	−0.302 (3)	0.3802 (13)	0.5476 (7)	0.090 (8)*
H9WB	−0.358 (3)	0.3319 (8)	0.6078 (13)	0.100 (9)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O4	0.0439 (6)	0.0355 (5)	0.0506 (6)	−0.0020 (4)	0.0200 (5)	−0.0028 (5)
O2	0.0563 (7)	0.0333 (6)	0.0528 (6)	0.0121 (5)	0.0187 (5)	0.0086 (5)
O1	0.0735 (8)	0.0375 (6)	0.0411 (6)	0.0100 (5)	0.0192 (5)	0.0112 (5)
O7	0.0802 (9)	0.0622 (8)	0.0472 (7)	0.0035 (7)	0.0254 (6)	0.0062 (6)
O3	0.0558 (7)	0.0379 (6)	0.0445 (6)	−0.0188 (5)	0.0165 (5)	−0.0095 (5)
O8	0.0799 (9)	0.0548 (8)	0.0619 (8)	−0.0041 (6)	0.0164 (7)	0.0222 (6)
N4	0.0553 (8)	0.0328 (6)	0.0353 (7)	0.0030 (5)	0.0038 (6)	−0.0046 (5)
N5	0.0414 (7)	0.0341 (7)	0.0400 (7)	0.0036 (5)	0.0093 (5)	0.0023 (5)
C1	0.0342 (7)	0.0271 (7)	0.0267 (6)	0.0014 (5)	0.0042 (5)	0.0002 (5)
C5	0.0335 (7)	0.0272 (7)	0.0317 (7)	0.0031 (5)	0.0064 (5)	0.0003 (5)
O6	0.0455 (7)	0.0771 (9)	0.0840 (10)	0.0088 (7)	−0.0164 (7)	0.0045 (8)
N1	0.0419 (7)	0.0367 (7)	0.0590 (8)	0.0083 (6)	0.0114 (6)	0.0131 (6)
N7	0.0424 (7)	0.0408 (7)	0.0352 (6)	0.0059 (5)	0.0086 (5)	−0.0018 (5)
N2	0.0640 (9)	0.0340 (7)	0.0374 (7)	−0.0006 (6)	0.0153 (6)	−0.0025 (5)
C6	0.0337 (7)	0.0244 (6)	0.0247 (6)	−0.0016 (5)	0.0049 (5)	−0.0023 (5)
N6	0.0464 (7)	0.0322 (6)	0.0452 (7)	−0.0007 (5)	0.0177 (6)	−0.0027 (5)
N3	0.0438 (7)	0.0333 (6)	0.0334 (6)	0.0011 (5)	0.0052 (5)	−0.0034 (5)
O5	0.0613 (8)	0.0378 (7)	0.1471 (15)	0.0172 (6)	0.0299 (9)	0.0047 (8)
C2	0.0308 (7)	0.0379 (8)	0.0388 (8)	0.0019 (6)	0.0050 (6)	0.0017 (6)
C14	0.0377 (7)	0.0343 (7)	0.0298 (7)	0.0011 (6)	−0.0026 (6)	−0.0021 (6)
C4	0.0458 (8)	0.0231 (6)	0.0418 (8)	−0.0001 (6)	0.0133 (6)	0.0031 (6)
C8	0.0330 (7)	0.0298 (7)	0.0317 (7)	−0.0012 (5)	0.0037 (5)	0.0018 (5)
C3	0.0374 (8)	0.0354 (8)	0.0445 (8)	−0.0078 (6)	0.0130 (6)	0.0005 (6)
C7	0.0357 (7)	0.0311 (7)	0.0344 (7)	0.0015 (6)	0.0023 (6)	0.0048 (6)
C9	0.0486 (9)	0.0593 (10)	0.0334 (8)	0.0110 (8)	0.0093 (7)	0.0081 (7)
C11	0.0293 (7)	0.0360 (7)	0.0347 (7)	0.0029 (5)	0.0020 (5)	−0.0006 (6)
C10	0.0438 (9)	0.0494 (9)	0.0404 (8)	0.0025 (7)	0.0039 (7)	0.0123 (7)
C13	0.0460 (8)	0.0488 (9)	0.0322 (8)	0.0065 (7)	0.0036 (6)	−0.0006 (7)
C15	0.0487 (9)	0.0476 (9)	0.0517 (9)	0.0067 (7)	0.0064 (7)	−0.0135 (8)
C12	0.0629 (10)	0.0468 (9)	0.0350 (8)	0.0098 (8)	0.0073 (7)	−0.0077 (7)
C16	0.0952 (15)	0.0345 (9)	0.0512 (10)	−0.0020 (9)	0.0069 (9)	−0.0022 (7)
O9W	0.1076 (11)	0.0374 (7)	0.0546 (8)	0.0013 (7)	0.0266 (8)	−0.0016 (6)

Geometric parameters (Å, º)

O4—C8	1.2491 (16)	C6—C8	1.5159 (18)
O2—C7	1.2458 (17)	N6—C11	1.2970 (18)
O1—C7	1.2508 (17)	N6—H6A	0.8600
O7—C13	1.2065 (19)	N6—H6B	0.8600
O3—C8	1.2459 (17)	N3—C14	1.3573 (19)
O8—C10	1.2072 (19)	N3—C13	1.3690 (19)

N4—C14	1.3232 (18)	N3—H3A	0.8600
N4—C16	1.443 (2)	C2—C3	1.380 (2)
N4—C12	1.450 (2)	C2—H2	0.9300
N5—C11	1.3617 (18)	C4—C3	1.379 (2)
N5—C10	1.369 (2)	C4—H4	0.9300
N5—H5	0.8600	C3—H3	0.9300
C1—C2	1.3911 (19)	C9—C10	1.507 (2)
C1—C6	1.3957 (18)	C9—H9A	0.9700
C1—C7	1.5070 (18)	C9—H9B	0.9700
C5—C4	1.3775 (19)	C13—C12	1.509 (2)
C5—C6	1.3836 (18)	C15—H15A	0.9600
C5—N1	1.4587 (18)	C15—H15B	0.9600
O6—N1	1.2200 (19)	C15—H15C	0.9600
N1—O5	1.2161 (18)	C12—H12A	0.9700
N7—C11	1.3311 (18)	C12—H12B	0.9700
N7—C15	1.452 (2)	C16—H16A	0.9600
N7—C9	1.452 (2)	C16—H16B	0.9600
N2—C14	1.3028 (19)	C16—H16C	0.9600
N2—H2A	0.8600	O9W—H9WA	0.855 (9)
N2—H2B	0.8600	O9W—H9WB	0.852 (9)

C14—N4—C16	127.06 (14)	O4—C8—C6	115.68 (12)
C14—N4—C12	109.84 (12)	C4—C3—C2	120.23 (13)
C16—N4—C12	123.07 (13)	C4—C3—H3	119.9
C11—N5—C10	110.75 (12)	C2—C3—H3	119.9
C11—N5—H5	124.6	O2—C7—O1	125.96 (13)
C10—N5—H5	124.6	O2—C7—C1	117.35 (12)
C2—C1—C6	120.02 (12)	O1—C7—C1	116.65 (12)
C2—C1—C7	119.63 (12)	N7—C9—C10	103.02 (12)
C6—C1—C7	120.29 (11)	N7—C9—H9A	111.2
C4—C5—C6	123.75 (12)	C10—C9—H9A	111.2
C4—C5—N1	117.95 (12)	N7—C9—H9B	111.2
C6—C5—N1	118.29 (12)	C10—C9—H9B	111.2
O5—N1—O6	123.96 (15)	H9A—C9—H9B	109.1
O5—N1—C5	118.51 (14)	N6—C11—N7	127.13 (13)
O6—N1—C5	117.52 (13)	N6—C11—N5	122.26 (13)
C11—N7—C15	125.62 (13)	N7—C11—N5	110.61 (12)
C11—N7—C9	109.51 (12)	O8—C10—N5	125.80 (16)
C15—N7—C9	122.51 (13)	O8—C10—C9	128.18 (15)
C14—N2—H2A	120.0	N5—C10—C9	106.03 (13)
C14—N2—H2B	120.0	O7—C13—N3	126.04 (15)
H2A—N2—H2B	120.0	O7—C13—C12	128.05 (14)
C5—C6—C1	117.10 (12)	N3—C13—C12	105.90 (13)
C5—C6—C8	121.54 (12)	N7—C15—H15A	109.5
C1—C6—C8	121.27 (11)	N7—C15—H15B	109.5
C11—N6—H6A	120.0	H15A—C15—H15B	109.5
C11—N6—H6B	120.0	N7—C15—H15C	109.5
H6A—N6—H6B	120.0	H15A—C15—H15C	109.5

C14—N3—C13	110.74 (12)	H15B—C15—H15C	109.5
C14—N3—H3A	124.6	N4—C12—C13	102.71 (12)
C13—N3—H3A	124.6	N4—C12—H12A	111.2
C3—C2—C1	120.78 (13)	C13—C12—H12A	111.2
C3—C2—H2	119.6	N4—C12—H12B	111.2
C1—C2—H2	119.6	C13—C12—H12B	111.2
N2—C14—N4	127.26 (14)	H12A—C12—H12B	109.1
N2—C14—N3	121.98 (13)	N4—C16—H16A	109.5
N4—C14—N3	110.74 (12)	N4—C16—H16B	109.5
C5—C4—C3	118.06 (12)	H16A—C16—H16B	109.5
C5—C4—H4	121.0	N4—C16—H16C	109.5
C3—C4—H4	121.0	H16A—C16—H16C	109.5
O3—C8—O4	126.73 (13)	H16B—C16—H16C	109.5
O3—C8—C6	117.58 (12)	H9WA—O9W—H9WB	105.1 (14)
C4—C5—N1—O5	49.1 (2)	C1—C6—C8—O4	−117.14 (14)
C6—C5—N1—O5	−132.09 (15)	C5—C4—C3—C2	−2.1 (2)
C4—C5—N1—O6	−131.17 (15)	C1—C2—C3—C4	2.6 (2)
C6—C5—N1—O6	47.61 (19)	C2—C1—C7—O2	55.03 (18)
C4—C5—C6—C1	1.80 (19)	C6—C1—C7—O2	−127.68 (14)
N1—C5—C6—C1	−176.91 (12)	C2—C1—C7—O1	−123.06 (15)
C4—C5—C6—C8	−174.78 (13)	C6—C1—C7—O1	54.23 (18)
N1—C5—C6—C8	6.51 (19)	C11—N7—C9—C10	−2.97 (16)
C2—C1—C6—C5	−1.31 (19)	C15—N7—C9—C10	−166.41 (14)
C7—C1—C6—C5	−178.58 (12)	C15—N7—C11—N6	−14.4 (2)
C2—C1—C6—C8	175.28 (12)	C9—N7—C11—N6	−177.21 (14)
C7—C1—C6—C8	−2.00 (18)	C15—N7—C11—N5	165.78 (14)
C6—C1—C2—C3	−0.8 (2)	C9—N7—C11—N5	2.98 (16)
C7—C1—C2—C3	176.46 (13)	C10—N5—C11—N6	178.51 (13)
C16—N4—C14—N2	1.0 (3)	C10—N5—C11—N7	−1.67 (17)
C12—N4—C14—N2	179.12 (15)	C11—N5—C10—O8	179.93 (16)
C16—N4—C14—N3	179.08 (16)	C11—N5—C10—C9	−0.30 (17)
C12—N4—C14—N3	−2.76 (17)	N7—C9—C10—O8	−178.31 (17)
C13—N3—C14—N2	−179.73 (14)	N7—C9—C10—N5	1.93 (16)
C13—N3—C14—N4	2.03 (16)	C14—N3—C13—O7	179.98 (16)
C6—C5—C4—C3	−0.1 (2)	C14—N3—C13—C12	−0.45 (16)
N1—C5—C4—C3	178.63 (13)	C14—N4—C12—C13	2.32 (17)
C5—C6—C8—O3	−121.68 (14)	C16—N4—C12—C13	−179.43 (15)
C1—C6—C8—O3	61.89 (17)	O7—C13—C12—N4	178.47 (16)
C5—C6—C8—O4	59.29 (17)	N3—C13—C12—N4	−1.08 (16)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O9*W*—H9*WA*···O2	0.86 (1)	1.94 (2)	2.7856 (18)	168 (2)
O9*W*—H9*WB*···O8^{i}	0.85 (1)	2.16 (2)	2.9241 (18)	149 (2)
N2—H2*A*···O3^{ii}	0.86	2.00	2.7899 (17)	152
N2—H2*B*···O2^{iii}	0.86	1.95	2.8000 (17)	168

N3—H3*A*···O1^{iii}	0.86	1.77	2.6275 (15)	177
N5—H5···O4^{iv}	0.86	1.84	2.6836 (16)	166
N6—H6*A*···O9*W*^{v}	0.86	1.96	2.7952 (17)	163
N6—H6*B*···O3^{iv}	0.86	1.94	2.7900 (16)	171
C4—H4···O5^{i}	0.93	2.59	3.2071 (19)	124
C9—H9*B*···O6^{vi}	0.97	2.47	3.212 (2)	133

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