Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-Amino-4,6-dimethylpyrimidinium 3,5-dinitrobenzoate dihydrate

Annamalai Subashini,[a] Packianathan Thomas Muthiah[a]* and Daniel E. Lynch[b]

[a]School of Chemistry, Bharathidasan University, Tiruchirappalli 620 024, Tamil Nadu, India, and [b]Faculty of Health and Life Sciences, Coventry University, Priory Street, Coventry CV1 5FB, England
Correspondence e-mail: tommtrichy@yahoo.co.in

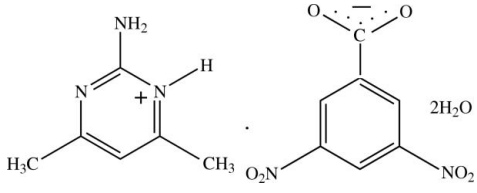
Received 21 November 2007; accepted 7 January 2008

Key indicators: single-crystal X-ray study; T = 120 K; mean σ(C–C) = 0.003 Å; R factor = 0.060; wR factor = 0.171; data-to-parameter ratio = 13.6.

In the title compound, $C_6H_{10}N_3^+\cdot C_7H_3N_2O_6^-\cdot 2H_2O$, the aminopyrimidine molecule is protonated at one of the pyrimidine N atoms. The carboxylate group of the 3,5-dinitrobenzoate anion interacts with the protonated pyrimidine N atom and the 2-amino group through a pair of N—H···O hydrogen bonds, forming an $R_2^2(8)$ motif. Two inversion-related pyrimidine rings are linked *via* a pair of N—H···N hydrogen bonds, also forming an $R_2^2(8)$ ring motif.

Related literature

For related literature, see: Allen *et al.* (1998); Baker & Santi (1965); Baskar Raj *et al.* (2003); Desiraju (1989); Hunt *et al.* (1980); Lynch & Jones (2004); Panneerselvam *et al.* (2004); Prince *et al.* (1991); Stanley *et al.* (2005); Subashini *et al.* (2006).



Experimental

Crystal data

$C_6H_{10}N_3^+\cdot C_7H_3N_2O_6^-\cdot 2H_2O$
M_r = 371.32
Triclinic, $P\overline{1}$
a = 7.1465 (3) Å
b = 11.0215 (5) Å
c = 11.1531 (4) Å
α = 99.473 (3)°
β = 101.322 (3)°
γ = 100.826 (2)°
V = 827.33 (6) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.13 mm^{-1}
T = 120 K
0.44 × 0.36 × 0.23 mm

Data collection

Bruker–Nonius KappaCCD area-detector diffractometer
Absorption correction: none
15739 measured reflections
3235 independent reflections
2283 reflections with $I > 2\sigma(I)$
R_{int} = 0.043

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.171
S = 1.04
3235 reflections
238 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.50 e Å^{-3}
$\Delta\rho_{min}$ = −0.55 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1	0.88	1.73	2.605 (3)	174
N2—H2A···N3^{i}	0.88	2.17	3.041 (3)	172
N2—H2B···O2	0.88	1.92	2.787 (3)	168

Symmetry code: (i) $-x, -y+1, -z+1$.

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

AS thanks Bharathidasan University for the award of a Research Student Fellowship (Reference CCCD/PhD-2/15504/2004). DEL thanks the EPSRC National Crystallography Service (Southampton, England) for the X-ray data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ2189).

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  doi:10.1107/S1600536808000524

supporting information

Acta Cryst. (2008). E**64**, o426 [doi:10.1107/S1600536808000524]

2-Amino-4,6-dimethylpyrimidinium 3,5-dinitrobenzoate dihydrate

Annamalai Subashini, Packianathan Thomas Muthiah and Daniel E. Lynch

S1. Comment

Hydrogen-bonding patterns involving aminopyrimidine and carboxylates have been observed in drug–receptor interactions, protein–nucleic acid interactions and supramolecular architectures (Desiraju, 1989). Studies of such interactions are also of current interest because of their applications in drug design and the crystal engineering of pharmaceuticals (Stanley *et al.*, 2005). Pyrimidine and aminopyrimidine derivatives are biologically important compounds as they occur in nature as components of nucleic acids. Some aminopyrimidine derivatives are used as antifolate drugs (Hunt *et al.*, 1980; Baker & Santi, 1965). Two monoclinic polymorphic forms of 3,5-dinitrobenzoic acid (Prince *et al.*, 1991) have already been reported. From our laboratory, the crystal structures of 2-amino-4,6-dimethyl-pyrimidinium bromide 2-amino-4,6-dimethyl pyrimidine monohydrate (Panneerselvam *et al.*, 2004) and 2-amino-4,6-dimethylpyrimidinium picrate (Subashini *et al.*, 2006) have been reported. The present study was undertaken to explore the hydrogen-bonding patterns involving aminopyrimidine–carboxylate interactions.

The asymmetric unit of the title compound contains one 2-amino-4,6-dimethylpyrimidinium cation, one 3,5-dinitro-benzoate anion and two water molecules (Fig. 1). Protonation of the pyrimidine base on the N1 site is reflected in a change in bond angle. The C2—N3—C4 angle at unprotonated atom N3 is 117.6 (2)°, while for protonated atom N1, the C2—N1—C6 angle is 120.5 (2)°. The carboxylate group of the 3,5-dinitrobenzoate anion (O1 and O2) interacts with the protonated N1 atom and the 2-amino group of the pyrimidine moiety through a pair of N—H···O hydrogen bonds, forming a fork-like interaction with graph-set $R_2^2(8)$ (Lynch & Jones, 2004). This $R_2^2(8)$ motif is one of the 24 most frequently observed bimolecular cyclic hydrogen-bonded motifs in organic crystal structures (Allen *et al.*, 1998). The aminopyrimidinium cations are centrosymmetrically paired through two N—H···N hydrogen hydrogen bonds involving the 2-amino group and the N3 nitrogen atom (graph-set $R_2^2(8)$) (Fig. 2). A similar type of interaction has been observed in crystal structure of trimethoprim *m*-chlorobenzoate and trimethoprim *m*-chlorobenzoate dihydrate (Baskar Raj *et al.*, 2003).

S2. Experimental

A hot ethanol solution of 2-amino-4,6-dimethylpyrimidine (31 mg, Aldrich) was added to a hot aqueous solution of 3,5-dinitrobenzoic acid (53 mg, LOBA) in a 1:1 molar ratio. The resultant solution was warmed over a water bath for an hour. After a few days brown colored block shaped crystals were obtained as a result of slow evaporation.

S3. Refinement

All H atoms were placed in idealized locations and were refined using a riding model, with C—H = 0.95–0.99 Å, N—H = 0.88 Å and U_{iso}(H) = 1.2 U_{eq}(C, N). The thermal parameters of both water molecules are very high. All the H atoms of the water molecules have been fixed and were not refined.

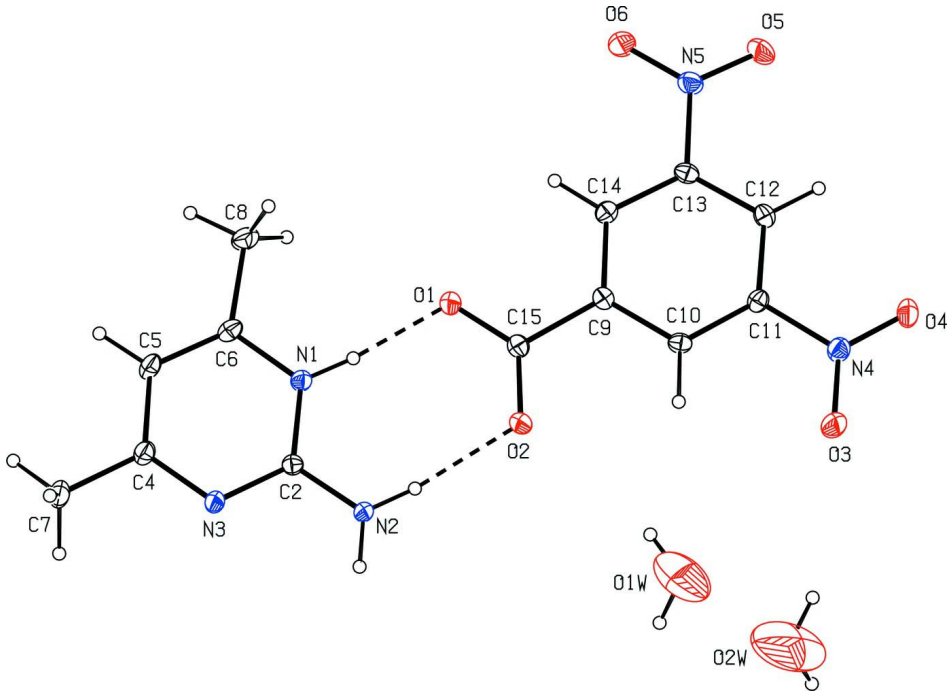

Figure 1

An *ORTEP* view of the asymmetric unit of the title compound showing 30% probability displacement ellipsoids. Hydrogen bonds are shown as dashed lines.

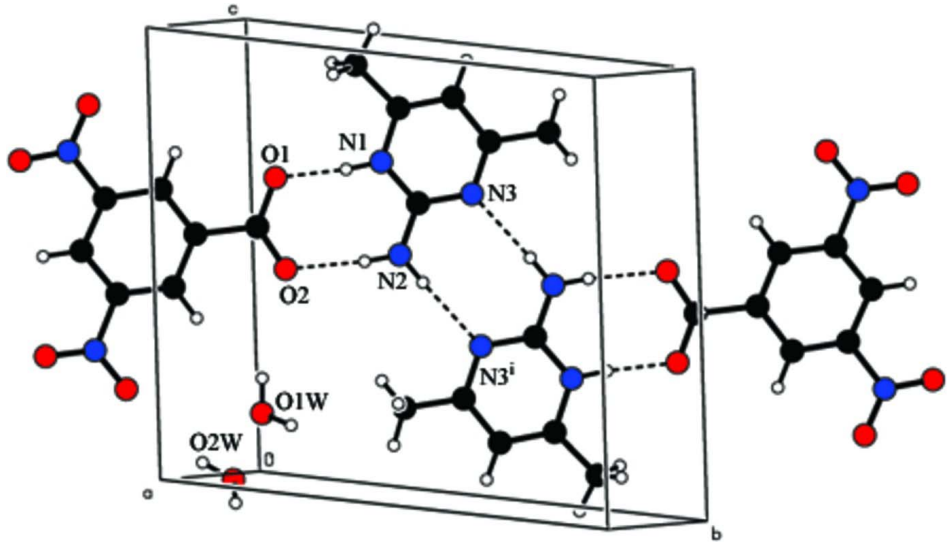

Figure 2

Hydrogen bonding patterns in the title compound. Symmetry codes: (i) -*x*, -*y* + 1, -*z* + 1.

2-Amino-4,6-dimethylpyrimidinium 3,5-dinitrobenzoate dihydrate

Crystal data

$C_6H_{10}N_3^+\cdot C_7H_3N_2O_6^-\cdot 2H_2O$
M_r = 371.32
Triclinic, $P\overline{1}$

Hall symbol: -P 1
a = 7.1465 (3) Å
b = 11.0215 (5) Å

c = 11.1531 (4) Å
α = 99.473 (3)°
β = 101.322 (3)°
γ = 100.826 (2)°
V = 827.33 (6) Å^3
Z = 2
F(000) = 388
D_x = 1.491 Mg m^{-3}

Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2.5 reflections
θ = 3.8–26.0°
μ = 0.13 mm^{-1}
T = 120 K
Block, brown
0.44 × 0.36 × 0.23 mm

Data collection

Bruker–Nonius KappaCCD area-detector diffractometer
Radiation source: Bruker–Nonius FR591 rotating anode
Graphite monochromator
φ and ω scans
15739 measured reflections

3235 independent reflections
2283 reflections with $I > 2\sigma(I)$
R_{int} = 0.043
θ_{max} = 26.0°, θ_{min} = 3.8°
h = −8→8
k = −13→13
l = −13→13

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.171
S = 1.04
3235 reflections
238 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0801P)^2 + 0.6543P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.50 e Å^{-3}
$\Delta\rho_{min}$ = −0.55 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001Fc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.026 (9)

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All e.s.d.'s are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted R-factors wR and all goodnesses 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 observed criterion of $F^2 > \sigma(F^2)$ is used only for calculating -R-factor-obs *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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
N1	0.2027 (3)	0.33914 (19)	0.72583 (18)	0.0274 (6)
N2	0.1151 (3)	0.35467 (18)	0.51987 (17)	0.0283 (6)
N3	0.0823 (3)	0.51366 (18)	0.67131 (17)	0.0284 (6)
C2	0.1339 (3)	0.4032 (2)	0.6397 (2)	0.0255 (7)
C4	0.1050 (4)	0.5608 (2)	0.7929 (2)	0.0316 (7)
C5	0.1819 (4)	0.4998 (2)	0.8853 (2)	0.0344 (8)
C6	0.2299 (4)	0.3872 (2)	0.8500 (2)	0.0321 (8)
C7	0.0403 (4)	0.6801 (3)	0.8255 (2)	0.0434 (9)

C8	0.3079 (4)	0.3114 (3)	0.9388 (2)	0.0425 (9)
O1	0.2748 (3)	0.11664 (16)	0.66737 (15)	0.0340 (5)
O2	0.1737 (3)	0.11087 (15)	0.46282 (15)	0.0330 (5)
O3	0.2112 (3)	−0.24607 (19)	0.15879 (17)	0.0491 (7)
O4	0.3323 (3)	−0.39796 (18)	0.21663 (17)	0.0432 (6)
O5	0.5402 (3)	−0.39570 (18)	0.65403 (19)	0.0467 (7)
O6	0.4999 (3)	−0.2476 (2)	0.79214 (18)	0.0545 (8)
N4	0.2803 (3)	−0.2987 (2)	0.23984 (19)	0.0335 (7)
N5	0.4871 (3)	−0.2986 (2)	0.6838 (2)	0.0355 (7)
C9	0.2796 (3)	−0.0654 (2)	0.5226 (2)	0.0258 (7)
C10	0.2515 (3)	−0.1244 (2)	0.3983 (2)	0.0271 (7)
C11	0.3026 (3)	−0.2394 (2)	0.3714 (2)	0.0275 (7)
C12	0.3787 (3)	−0.3000 (2)	0.4618 (2)	0.0285 (7)
C13	0.4021 (3)	−0.2388 (2)	0.5846 (2)	0.0284 (7)
C14	0.3543 (3)	−0.1233 (2)	0.6170 (2)	0.0279 (7)
C15	0.2368 (3)	0.0642 (2)	0.5522 (2)	0.0282 (7)
O1W	0.0473 (17)	0.0204 (5)	0.1315 (8)	0.279 (6)
O2W	0.229 (3)	−0.0073 (6)	−0.0151 (9)	0.474 (10)
H1	0.23000	0.26580	0.70130	0.0330*
H2A	0.06960	0.39440	0.46230	0.0340*
H2B	0.14830	0.28270	0.49790	0.0340*
H5	0.20050	0.53630	0.97130	0.0410*
H7A	0.08110	0.73780	0.77250	0.0650*
H7B	0.09990	0.71960	0.91350	0.0650*
H7C	−0.10280	0.66140	0.81180	0.0650*
H8A	0.20720	0.23550	0.93330	0.0640*
H8B	0.34390	0.36210	1.02420	0.0640*
H8C	0.42380	0.28660	0.91730	0.0640*
H10	0.19820	−0.08650	0.33280	0.0320*
H12	0.41290	−0.37870	0.44120	0.0340*
H14	0.37250	−0.08460	0.70240	0.0330*
H1W	0.08570	0.03120	0.21100	0.5000*
H2W	0.08640	0.09280	0.11360	0.5000*
H3W	0.27840	−0.06530	0.01730	0.5000*
H4W	0.31380	0.01390	−0.06280	0.5000*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0299 (11)	0.0296 (11)	0.0237 (10)	0.0107 (8)	0.0048 (8)	0.0057 (8)
N2	0.0387 (11)	0.0276 (11)	0.0201 (10)	0.0132 (9)	0.0051 (8)	0.0048 (8)
N3	0.0335 (11)	0.0288 (11)	0.0224 (10)	0.0102 (9)	0.0049 (8)	0.0023 (8)
C2	0.0258 (12)	0.0260 (12)	0.0247 (12)	0.0069 (9)	0.0044 (9)	0.0057 (9)
C4	0.0340 (13)	0.0349 (13)	0.0242 (12)	0.0086 (11)	0.0057 (10)	0.0019 (10)
C5	0.0377 (14)	0.0418 (15)	0.0210 (12)	0.0098 (12)	0.0052 (10)	−0.0002 (11)
C6	0.0310 (13)	0.0429 (15)	0.0223 (12)	0.0089 (11)	0.0044 (10)	0.0079 (11)
C7	0.0584 (18)	0.0442 (16)	0.0293 (14)	0.0246 (14)	0.0089 (13)	−0.0008 (12)
C8	0.0509 (17)	0.0532 (17)	0.0275 (13)	0.0204 (14)	0.0061 (12)	0.0137 (12)

O1	0.0443 (10)	0.0293 (9)	0.0276 (9)	0.0117 (8)	0.0058 (8)	0.0034 (7)
O2	0.0418 (10)	0.0282 (9)	0.0306 (9)	0.0130 (8)	0.0058 (7)	0.0081 (7)
O3	0.0682 (14)	0.0540 (13)	0.0280 (10)	0.0282 (11)	0.0047 (9)	0.0079 (9)
O4	0.0543 (12)	0.0393 (11)	0.0371 (10)	0.0195 (9)	0.0120 (9)	−0.0005 (8)
O5	0.0540 (12)	0.0408 (11)	0.0513 (12)	0.0265 (10)	0.0066 (9)	0.0150 (9)
O6	0.0819 (16)	0.0477 (12)	0.0293 (11)	0.0239 (11)	−0.0054 (10)	0.0069 (9)
N4	0.0348 (12)	0.0362 (12)	0.0286 (11)	0.0105 (10)	0.0052 (9)	0.0038 (9)
N5	0.0394 (12)	0.0330 (12)	0.0334 (12)	0.0108 (10)	0.0018 (9)	0.0098 (9)
C9	0.0220 (11)	0.0244 (12)	0.0295 (12)	0.0042 (9)	0.0043 (9)	0.0045 (10)
C10	0.0237 (12)	0.0293 (13)	0.0274 (12)	0.0055 (10)	0.0019 (9)	0.0093 (10)
C11	0.0253 (12)	0.0314 (13)	0.0245 (12)	0.0063 (10)	0.0050 (9)	0.0034 (10)
C12	0.0261 (12)	0.0261 (12)	0.0333 (13)	0.0078 (10)	0.0060 (10)	0.0049 (10)
C13	0.0245 (12)	0.0291 (12)	0.0317 (13)	0.0068 (10)	0.0020 (10)	0.0110 (10)
C14	0.0257 (12)	0.0301 (13)	0.0260 (12)	0.0039 (10)	0.0047 (9)	0.0048 (10)
C15	0.0259 (12)	0.0271 (12)	0.0318 (13)	0.0065 (10)	0.0072 (10)	0.0057 (10)
O1W	0.516 (15)	0.093 (4)	0.240 (8)	0.075 (6)	0.084 (9)	0.065 (4)
O2W	1.00 (3)	0.072 (3)	0.178 (6)	−0.018 (11)	−0.117 (16)	0.013 (4)

Geometric parameters (Å, º)

O1—C15	1.272 (3)	C4—C7	1.487 (4)
O2—C15	1.241 (3)	C5—C6	1.366 (3)
O3—N4	1.226 (3)	C6—C8	1.490 (4)
O4—N4	1.224 (3)	C5—H5	0.9499
O5—N5	1.218 (3)	C7—H7C	0.9802
O6—N5	1.224 (3)	C7—H7A	0.9801
O1W—H1W	0.8562	C7—H7B	0.9797
O1W—H2W	0.8633	C8—H8B	0.9799
O2W—H4W	0.9051	C8—H8C	0.9797
O2W—H3W	0.8801	C8—H8A	0.9803
N1—C2	1.353 (3)	C9—C14	1.389 (3)
N1—C6	1.360 (3)	C9—C15	1.514 (3)
N2—C2	1.326 (3)	C9—C10	1.389 (3)
N3—C2	1.349 (3)	C10—C11	1.386 (3)
N3—C4	1.336 (3)	C11—C12	1.379 (3)
N1—H1	0.8796	C12—C13	1.386 (3)
N2—H2B	0.8804	C13—C14	1.389 (3)
N2—H2A	0.8797	C10—H10	0.9509
N4—C11	1.469 (3)	C12—H12	0.9492
N5—C13	1.468 (3)	C14—H14	0.9502
C4—C5	1.400 (3)		
O1···N1	2.605 (3)	C9···C10^{i}	3.461 (3)
O1···C8	3.349 (3)	C9···O2^{iii}	3.224 (3)
O1···C11^{i}	3.211 (3)	C9···C9^{i}	3.378 (3)
O1W···O2W	2.30 (2)	C10···C14^{i}	3.588 (3)
O1W···O1W^{ii}	2.817 (12)	C10···C9^{i}	3.461 (3)
O1W···O2W^{ii}	2.10 (2)	C10···C15^{i}	3.506 (3)

O2···N2	2.787 (3)	C11···C2^{iii}	3.266 (3)
O2···C15^{iii}	3.151 (3)	C11···O1^{i}	3.211 (3)
O2···C9^{iii}	3.224 (3)	C11···C15^{i}	3.355 (3)
O2···C12^{i}	3.339 (3)	C12···O2^{i}	3.339 (3)
O2···C13^{i}	3.275 (3)	C12···C15^{i}	3.457 (3)
O2W···O1W^{ii}	2.10 (2)	C12···C2^{iii}	3.518 (3)
O2W···O1W	2.30 (2)	C13···O2^{i}	3.275 (3)
O3···C6^{iii}	3.218 (4)	C14···C10^{i}	3.588 (3)
O4···O5^{iv}	3.070 (3)	C15···N1	3.395 (3)
O4···C4^{iii}	3.271 (3)	C15···C10^{i}	3.506 (3)
O4···C6^{i}	3.340 (4)	C15···C11^{i}	3.355 (3)
O4···N1^{i}	3.177 (3)	C15···C12^{i}	3.457 (3)
O5···C2^{v}	3.264 (3)	C15···C15^{iii}	3.305 (3)
O5···O4^{iv}	3.070 (3)	C15···O2^{iii}	3.151 (3)
O6···C8^{vi}	3.290 (3)	C4···H2A^{x}	3.0334
O6···C7^{v}	3.340 (4)	C7···H2W^{x}	2.8424
O6···C4^{v}	3.194 (3)	C7···H2A^{x}	3.0813
O1···H1	1.7288	C15···H1	2.5614
O1···H14	2.5138	C15···H2B	2.7328
O1W···H3W^{ii}	2.7574	H1···H8C	2.4826
O1W···H3W	2.5016	H1···O1	1.7288
O1W···H2W^{ii}	2.7104	H1···O2	2.8247
O1W···H10	2.8265	H1···C15	2.5614
O1W···H4W^{ii}	2.4802	H1···H2B	2.2763
O2···H1	2.8247	H1W···H10	2.1720
O2···H2B	1.9198	H1W···O2W	2.9005
O2···H10	2.4637	H1W···O2	2.7096
O2···H1W	2.7096	H1W···O2W^{ii}	2.7495
O2W···H8A^{vii}	2.8539	H2A···C4^{x}	3.0334
O2W···H1W	2.9005	H2A···C7^{x}	3.0813
O2W···H2W^{ii}	2.2504	H2A···N3^{x}	2.1682
O2W···H2W	2.1890	H2B···O2	1.9198
O2W···H7B^{viii}	2.9025	H2B···H1	2.2763
O2W···H1W^{ii}	2.7495	H2B···C15	2.7328
O3···H3W	2.7683	H2W···O1W^{ii}	2.7104
O3···H5^{viii}	2.8895	H2W···C7^{x}	2.8424
O3···H7B^{viii}	2.6367	H2W···O2W	2.1890
O3···H10	2.4242	H2W···O2W^{ii}	2.2504
O4···H8C^{i}	2.7564	H3W···H7B^{viii}	2.4431
O4···H5^{viii}	2.6416	H3W···O1W	2.5016
O4···H12	2.4213	H3W···O1W^{ii}	2.7574
O5···H12^{iv}	2.6470	H3W···O3	2.7683
O5···H12	2.4207	H4W···O1W^{ii}	2.4802
O5···H7C^{ix}	2.6965	H5···H8B	2.4411
O6···H14	2.4304	H5···H7B	2.4096
O6···H8B^{vi}	2.7417	H5···O4^{xii}	2.6416
N1···O4^{i}	3.177 (3)	H5···O3^{xii}	2.8895
N1···O1	2.605 (3)	H7B···O2W^{xii}	2.9025

N1···C15	3.395 (3)	H7B···O3^{xii}	2.6367
N2···N3^{x}	3.041 (3)	H7B···H5	2.4096
N2···O2	2.787 (3)	H7B···H3W^{xii}	2.4431
N3···N2^{x}	3.041 (3)	H7C···O5^{xiii}	2.6965
N3···N5^{xi}	3.189 (3)	H8A···O2W^{xiv}	2.8539
N5···C4^{v}	3.417 (3)	H8B···O6^{vi}	2.7417
N5···N3^{v}	3.189 (3)	H8B···H5	2.4411
N3···H2A^{x}	2.1682	H8C···H1	2.4826
C2···C12^{iii}	3.518 (3)	H8C···O4^{i}	2.7564
C2···C11^{iii}	3.266 (3)	H10···O2	2.4637
C2···O5^{xi}	3.264 (3)	H10···O3	2.4242
C4···N5^{xi}	3.417 (3)	H10···O1W	2.8265
C4···O6^{xi}	3.194 (3)	H10···H1W	2.1720
C4···O4^{iii}	3.271 (3)	H12···O5^{iv}	2.6470
C6···O3^{iii}	3.218 (4)	H12···O5	2.4207
C6···O4^{i}	3.340 (4)	H12···O4	2.4213
C7···O6^{xi}	3.340 (4)	H14···O6	2.4304
C8···O6^{vi}	3.290 (3)	H14···O1	2.5138
C8···O1	3.349 (3)		

H1W—O1W—H2W	105.95	H7B—C7—H7C	109.53
H3W—O2W—H4W	100.59	C4—C7—H7B	109.45
C2—N1—C6	120.5 (2)	C4—C7—H7A	109.44
C2—N3—C4	117.6 (2)	H8B—C8—H8C	109.45
C6—N1—H1	119.74	C6—C8—H8B	109.50
C2—N1—H1	119.71	C6—C8—H8A	109.44
H2A—N2—H2B	119.98	H8A—C8—H8C	109.41
C2—N2—H2B	119.99	H8A—C8—H8B	109.50
C2—N2—H2A	120.02	C6—C8—H8C	109.53
O3—N4—C11	118.3 (2)	C10—C9—C15	118.94 (19)
O4—N4—C11	118.4 (2)	C14—C9—C15	121.27 (19)
O3—N4—O4	123.3 (2)	C10—C9—C14	119.7 (2)
O6—N5—C13	117.7 (2)	C9—C10—C11	118.9 (2)
O5—N5—C13	118.5 (2)	N4—C11—C12	117.9 (2)
O5—N5—O6	123.8 (2)	N4—C11—C10	118.59 (19)
N1—C2—N3	122.4 (2)	C10—C11—C12	123.5 (2)
N1—C2—N2	118.5 (2)	C11—C12—C13	115.8 (2)
N2—C2—N3	119.0 (2)	N5—C13—C14	119.25 (19)
C5—C4—C7	121.4 (2)	C12—C13—C14	123.1 (2)
N3—C4—C7	116.7 (2)	N5—C13—C12	117.6 (2)
N3—C4—C5	121.8 (2)	C9—C14—C13	118.9 (2)
C4—C5—C6	119.1 (2)	O1—C15—C9	116.30 (19)
N1—C6—C5	118.5 (2)	O1—C15—O2	126.1 (2)
C5—C6—C8	124.3 (2)	O2—C15—C9	117.57 (19)
N1—C6—C8	117.2 (2)	C11—C10—H10	120.58
C6—C5—H5	120.51	C9—C10—H10	120.55
C4—C5—H5	120.44	C11—C12—H12	122.06
H7A—C7—H7C	109.42	C13—C12—H12	122.12

H7A—C7—H7B	109.53	C13—C14—H14	120.45
C4—C7—H7C	109.45	C9—C14—H14	120.62
C6—N1—C2—N2	178.0 (2)	C4—C5—C6—C8	−178.4 (3)
C6—N1—C2—N3	−2.6 (4)	C4—C5—C6—N1	0.6 (4)
C2—N1—C6—C5	1.5 (4)	C14—C9—C10—C11	−1.2 (3)
C2—N1—C6—C8	−179.4 (2)	C15—C9—C10—C11	175.9 (2)
C4—N3—C2—N1	1.3 (4)	C10—C9—C14—C13	0.9 (3)
C4—N3—C2—N2	−179.3 (2)	C15—C9—C14—C13	−176.1 (2)
C2—N3—C4—C5	0.9 (4)	C10—C9—C15—O1	−176.4 (2)
C2—N3—C4—C7	−177.8 (2)	C10—C9—C15—O2	1.6 (3)
O4—N4—C11—C12	−0.9 (3)	C14—C9—C15—O1	0.7 (3)
O3—N4—C11—C10	−2.4 (3)	C14—C9—C15—O2	178.7 (2)
O4—N4—C11—C10	177.4 (2)	C9—C10—C11—N4	−177.5 (2)
O3—N4—C11—C12	179.4 (2)	C9—C10—C11—C12	0.7 (3)
O5—N5—C13—C14	−175.2 (2)	N4—C11—C12—C13	178.3 (2)
O5—N5—C13—C12	3.0 (3)	C10—C11—C12—C13	0.1 (3)
O6—N5—C13—C12	−176.9 (2)	C11—C12—C13—N5	−178.6 (2)
O6—N5—C13—C14	4.9 (3)	C11—C12—C13—C14	−0.4 (3)
N3—C4—C5—C6	−1.9 (4)	N5—C13—C14—C9	178.0 (2)
C7—C4—C5—C6	176.7 (3)	C12—C13—C14—C9	−0.1 (3)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1	0.88	1.73	2.605 (3)	174
N2—H2*A*···N3^{x}	0.88	2.17	3.041 (3)	172
N2—H2*B*···O2	0.88	1.92	2.787 (3)	168

Symmetry code: (x) −*x*, −*y*+1, −*z*+1.