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2,6-Diamino-5-(2,4-diamino-6-oxo-1,6-dihydropyrimidin-5-ylmethyl)-4-oxo-pyrimidin-1-ium 3,5-dinitrobenzoate

Annamalai Subashini,[a] Packianathan Thomas Muthiah,[a]* Gabriele Bocelli[b] and Andrea Cantoni[b]

[a]School of Chemistry, Bharathidasan University, Tiruchirappalli 620 024, Tamil Nadu, India, and [b]IMEM-CNR, Parco Area delle Scienze 37a, I-43010 Fontanini–Parma, Italy
Correspondence e-mail: tommtrichy@yahoo.co.in

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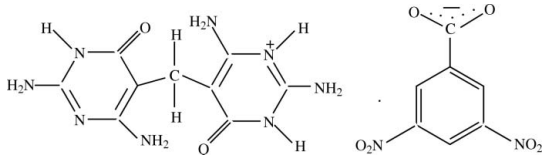
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.044; wR factor = 0.129; data-to-parameter ratio = 13.7.

In the title compound, $C_9H_{13}N_8O_2^+\cdot C_7H_3N_2O_6^-$, 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 N atom and the 2-amino group in a nearly linear fashion through a pair of N—H···O hydrogen bonds, generating the typical $R_2^2(8)$ motif. Two inversion-related pyrimidine units are connected through a pair of N—H···N hydrogen bonds, forming a cyclic hydrogen-bonded $R_2^2(8)$ motif. In addition to the base pairing, one of the carboxylate O atoms bridges the 4′-amino and 6′-amino groups on both side of the pairing, forming a *DADA* array. The molecular conformation of the cation is stabilized by two intramolecular N—H···O hydrogen bonds.

Related literature

For related literature, see: Allen *et al.* (1998); Baker & Santi (1965); Bernstein *et al.* (1995); Desiraju (1989); Etter (1990); Francis (2003); Hunt *et al.* (1980); Lynch & Jones (2004); Prince *et al.* (1991); Raj *et al.* (2003); Stanley *et al.* (2005); Subashini, Samuel *et al.* (2007); Subashini, Muthiah *et al.* (2007); Skoweranda *et al.* (1990).



Experimental

Crystal data

$C_9H_{13}N_8O_2^+\cdot C_7H_3N_2O_6^-$
M_r = 476.39
Monoclinic, $P2_1/n$
a = 7.365 (2) Å
b = 19.788 (3) Å
c = 13.658 (2) Å
β = 92.70 (2)°
V = 1988.3 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.13 mm^{-1}
T = 293 K
0.16 × 0.13 × 0.11 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: none
14081 measured reflections
4216 independent reflections
3046 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.129
S = 1.03
4216 reflections
307 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O2	0.86	1.81	2.663 (2)	173
N6′—H6A′···O3^{i}	0.86	2.06	2.867 (2)	156
N6′—H6B′···O1	0.86	2.09	2.929 (2)	166
N2—H2A···O3	0.86	1.95	2.781 (2)	163
N2—H2B···O1′^{ii}	0.86	2.27	2.991 (2)	141
N3—H3···O1′^{ii}	0.86	1.97	2.775 (2)	155
N3′—H3′···O6^{iii}	0.86	2.34	3.056 (2)	141
N4′—H4A′···N5′^{iv}	0.86	2.23	3.071 (2)	165
N4′—H4B′···O7^{iii}	0.86	2.56	3.355 (2)	154
N4′—H4B′···O3^{v}	0.86	2.53	3.136 (2)	129
N6—H6A···O1′	0.86	2.10	2.916 (2)	157
C7—H7A···O1	0.97	2.55	2.930 (2)	103
C7—H7B···O1′	0.97	2.55	2.925 (2)	103

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 2001); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2550).

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supplementary materials

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2,6-Diamino-5-(2,4-diamino-6-oxo-1,6-dihydropyrimidin-5-ylmethyl)-4-oxopyrimidin-1-ium 3,5-dinitrobenzoate

A. Subashini, P. T. Muthiah, G. Bocelli and A. Cantoni

Comment

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). 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). Two monoclinic polymorphic forms of 3,5-dinitrobenzoic acid (Prince *et al.*, 1991) have already been reported in literature. From our laboratory the crystal structures of trimethoprim (TMP) 3,5-dinitrobenzoate (Francis, 2003), TMP-3,5-dinitrosalicylate (Subashini, Samuel *et al.*, 2007) and pyrimethamine (PMN) 3,5-dinitrobenzoate (Subashini, Muthiah *et al.*, 2007) have been reported.

The asymmetric unit of the title compound contains a protonated 2,6-diamino-4-oxopyrimidinium −5-methylene-2'-oxo-4',6'-diaminopyrimidine (DAMPY) cation and a 3,5-dinitro benzoate anion (Fig.1). The DAMPY cation consists of one pyrimidinium cation and a neutral pyrimidine molecule bridged by a methylene group. The protonation at N1 of the pyrimidine moiety is evident from the increase in the internal angle at N1 (C2—N1—C6) from 116.4 (2)° in neutral 2,6-diamino-4(3*H*)-pyrimidinone monohydrate (Skoweranda *et al.*, 1990) to 121.02 (14)° in the present study. The carboxylate group (atoms O2 and O3) of the 3,5-dinitrobenzoate anion interact with the protonated atom N1 and the 2-amino group of the pyrimidine moiety through a pair of N—H···O hydrogen bonds, leading to the common ring motif with graph-set notation $R_2^2(8)$ (Lynch & Jones, 2004). This motif is reminiscent of the cyclic hydrogen-bonded motif occurring in the crystal structures of many aminopyrimidine carboxylates (Allen *et al.*, 1998; Raj *et al.*, 2003). Adjacent pyrimidinium cations are linked together by way of N—H···O bonds from the N3 and N2 amino donors to the O1' keto acceptor, resulting in chains containing $R^1_2(6)$ rings (Etter, 1990; Bernstein *et al.*, 1995). Two inversion related pyrimidine groups are paired centrosymmetrically through N4'-H4A'···N5'hydrogen bonds generating the $R_2^2(8)$ ring motif. In addition to the base-pairing, one of the carboxylate oxygen atoms (O3) bridges the 4'-amino and the 6'-amino groups on both sides of the pairing. This combination of base-pairing patterns and the further bridging of the bases leads to the formation of array of four hydrogen bonds. This is called a complementary DADA array of quadruple hydrogen bonding patterns (D = hydrogen bond donor and A = hydrogen bond acceptor) (Fig 2). The N3' atom and the 4'-amino group are hydrogen bonded to the oxygen atoms (O6 & O7) of the nitro group through a pair of N—H···O hydrogen bonds, generating the common $R_2^2(8)$ ring motif. The $R_2^2(8)$ motif is frequently observed in aminopyrimidine-carboxylate (Lynch & Jones, 2004) salts. Here, the nitro group mimics the role of carboxylate group. There is intramolecular hydrogen bonding between the N6/N6' amino groups and O1'/O1 keto groups. Further, N3' atom acts as a bifurcated donor to the nitro oxygen (O6 & O7) atoms. The combination of all types of intermolecular hydrogen bonds forms a three-dimensional network (Fig. 3).

Experimental

A hot methanol solution of 2,6-diamino-pyrimidin-4(3*H*)one (62 mg, Aldrich) was added to a hot aqueous solution of 3,5- dinitrobenzoic acid (53 mg, Aldrich) in a 2:1 molar ratio. A few drops of formaldehyde were added to the above solution. The resultant solution was warmed over a water bath for four hours. After a few days plate-like red crystals were obtained from the mother liquor.

Refinement

All hydrogen atoms were placed in idealized locations and refined as riding with C—H and N—H bond lengths of 0.97Å and 0.86 Å, respectively, and U(H) = 1.2U_{eq}(C,*N*).

Figures

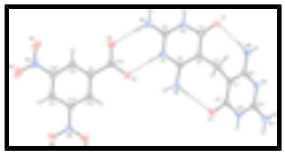


Fig. 1. An *ORTEP* diagram of the asymmetric unit of (I) showing 30% probability displacement ellipsoids.

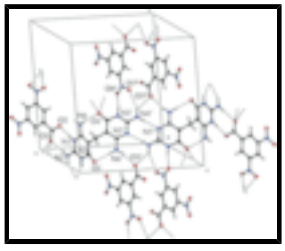


Fig. 2. View of DADA array in compound (I). Symmetry Codes: (i) −*x* + 1/2,*y* − 1/2,-*z* + 1/2; (iii) −*x* − 1/2,*y* − 1/2,-*z* − 1/2; (iv) −*x* + 1,-*y*,-*z*: (v) *x* + 1/2,-*y* + 1/2,*z* − 1/2.

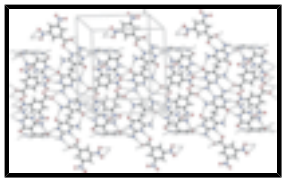


Fig. 3. Overall packing view of compound (I).

2,6-Diamino-5-(2,4-diamino-6-oxo-1,6-dihydropyrimidin-5-ylmethyl)-4- oxopyrimidin-1-ium 3,5-dinitrobenzoate

Crystal data

$C_9H_{13}N_8O_2^+ \cdot C_7H_3N_2O_6^-$	F_{000} = 984
M_r = 476.39	D_x = 1.591 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 25 reflections
a = 7.365 (2) Å	θ = 1.8–28.0º
b = 19.788 (3) Å	μ = 0.13 mm^{-1}
c = 13.658 (2) Å	*T* = 293 K

β = 92.70 (2)º	Plate-like, dark-red
V = 1988.3 (7) Å^3	0.16 × 0.13 × 0.11 mm
Z = 4	

Data collection

Bruker SMART CCD diffractometer	3046 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.027
Monochromator: graphite	θ_{max} = 28.0º
T = 293 K	θ_{min} = 1.8º
ω scans	h = −9→9
Absorption correction: none	k = −24→25
14081 measured reflections	l = −18→15
4216 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.044	H-atom parameters constrained
$wR(F^2)$ = 0.129	$w = 1/[\sigma^2(F_o^2) + (0.0811P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.03	$(\Delta/\sigma)_{max} < 0.001$
4216 reflections	$\Delta\rho_{max}$ = 0.30 e Å^{-3}
307 parameters	$\Delta\rho_{min}$ = −0.20 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > 2\text{sigma}(F^2)$ 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}
O1	0.14706 (18)	0.18678 (6)	0.35996 (9)	0.0561 (4)
O1'	−0.17937 (15)	0.13724 (6)	−0.02359 (9)	0.0505 (4)
N1	−0.02333 (17)	0.33870 (7)	0.18543 (10)	0.0427 (4)

N2	0.1212 (2)	0.41207 (8)	0.29440 (11)	0.0529 (5)
N3	0.13675 (19)	0.29771 (7)	0.32142 (10)	0.0466 (5)
N3'	0.07063 (18)	0.07452 (7)	−0.05341 (10)	0.0453 (4)
N4'	0.3125 (2)	0.00855 (8)	−0.09363 (11)	0.0544 (5)
N5'	0.29913 (18)	0.04685 (7)	0.06500 (10)	0.0434 (4)
N6	−0.1676 (2)	0.26934 (8)	0.07117 (11)	0.0559 (5)
N6'	0.2848 (2)	0.08959 (8)	0.21976 (11)	0.0537 (5)
C1'	0.0347 (2)	0.11346 (8)	0.10752 (11)	0.0394 (5)
C2	0.0773 (2)	0.34998 (8)	0.26789 (12)	0.0406 (5)
C2'	−0.0325 (2)	0.11055 (8)	0.01073 (12)	0.0412 (5)
C4	0.0916 (2)	0.23008 (9)	0.30063 (12)	0.0435 (5)
C4'	0.2293 (2)	0.04365 (8)	−0.02568 (12)	0.0416 (5)
C5	−0.0150 (2)	0.21896 (8)	0.21273 (12)	0.0410 (5)
C6	−0.0688 (2)	0.27348 (8)	0.15603 (12)	0.0410 (5)
C6'	0.2048 (2)	0.08402 (8)	0.13017 (12)	0.0409 (5)
C7	−0.0736 (2)	0.14767 (8)	0.18496 (12)	0.0442 (5)
O2	−0.16430 (17)	0.43773 (6)	0.07378 (9)	0.0530 (4)
O3	−0.07352 (19)	0.51100 (7)	0.18985 (10)	0.0636 (5)
O4	−0.1547 (3)	0.75282 (9)	0.12584 (16)	0.1066 (9)
O5	−0.3364 (3)	0.78625 (8)	0.00784 (15)	0.0989 (8)
O6	−0.5558 (2)	0.62731 (9)	−0.23607 (11)	0.0798 (6)
O7	−0.5115 (2)	0.52095 (8)	−0.21502 (10)	0.0656 (5)
N7	−0.2520 (3)	0.74235 (9)	0.05372 (15)	0.0695 (7)
N8	−0.4934 (2)	0.57961 (9)	−0.18840 (11)	0.0530 (5)
C8	−0.2224 (2)	0.55403 (8)	0.04574 (12)	0.0414 (5)
C9	−0.1993 (2)	0.62059 (9)	0.07690 (13)	0.0478 (6)
C10	−0.2749 (2)	0.67215 (9)	0.01992 (14)	0.0498 (6)
C11	−0.3740 (2)	0.66040 (9)	−0.06636 (13)	0.0499 (6)
C12	−0.3926 (2)	0.59391 (9)	−0.09554 (12)	0.0440 (5)
C13	−0.3183 (2)	0.54039 (9)	−0.04180 (12)	0.0417 (5)
C14	−0.1460 (2)	0.49614 (9)	0.10781 (13)	0.0450 (5)
H1	−0.06050	0.37240	0.15010	0.0510*
H6A'	0.38810	0.07050	0.23280	0.0640*
H6B'	0.23310	0.11220	0.26440	0.0640*
H2A	0.08240	0.44570	0.25950	0.0630*
H2B	0.18870	0.41890	0.34660	0.0630*
H3	0.20730	0.30580	0.37200	0.0560*
H3'	0.03240	0.07160	−0.11370	0.0540*
H4A'	0.41250	−0.01230	−0.07850	0.0650*
H4B'	0.26630	0.00670	−0.15260	0.0650*
H6A	−0.20180	0.23050	0.04880	0.0670*
H6B	−0.19680	0.30550	0.03920	0.0670*
H7A	−0.06640	0.12000	0.24360	0.0530*
H7B	−0.20010	0.14900	0.16180	0.0530*
H9	−0.13390	0.63020	0.13510	0.0570*
H11	−0.42590	0.69550	−0.10320	0.0600*
H13	−0.33240	0.49620	−0.06410	0.0500*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0745 (8)	0.0519 (7)	0.0404 (7)	0.0040 (6)	−0.0138 (6)	0.0025 (6)
O1'	0.0486 (6)	0.0573 (7)	0.0440 (7)	0.0097 (5)	−0.0154 (5)	0.0005 (5)
N1	0.0461 (7)	0.0411 (7)	0.0398 (8)	0.0077 (6)	−0.0082 (6)	−0.0018 (6)
N2	0.0595 (9)	0.0471 (9)	0.0504 (9)	0.0016 (7)	−0.0150 (7)	−0.0067 (7)
N3	0.0503 (8)	0.0503 (9)	0.0378 (8)	0.0013 (6)	−0.0127 (6)	−0.0040 (6)
N3'	0.0485 (7)	0.0545 (8)	0.0319 (7)	0.0044 (6)	−0.0075 (6)	−0.0021 (6)
N4'	0.0516 (8)	0.0698 (10)	0.0414 (8)	0.0093 (7)	−0.0032 (7)	−0.0080 (7)
N5'	0.0447 (7)	0.0439 (8)	0.0407 (8)	0.0034 (6)	−0.0073 (6)	−0.0019 (6)
N6	0.0668 (9)	0.0488 (8)	0.0498 (9)	0.0073 (7)	−0.0219 (7)	−0.0056 (7)
N6'	0.0576 (9)	0.0603 (10)	0.0417 (8)	0.0160 (7)	−0.0148 (7)	−0.0063 (7)
C1'	0.0431 (8)	0.0373 (8)	0.0369 (9)	0.0010 (6)	−0.0068 (7)	0.0010 (6)
C2	0.0380 (7)	0.0448 (9)	0.0388 (9)	0.0032 (6)	−0.0015 (6)	−0.0057 (7)
C2'	0.0438 (8)	0.0384 (8)	0.0408 (9)	−0.0014 (7)	−0.0057 (7)	0.0022 (7)
C4	0.0463 (9)	0.0481 (10)	0.0358 (9)	0.0041 (7)	−0.0018 (7)	−0.0014 (7)
C4'	0.0413 (8)	0.0412 (9)	0.0418 (9)	−0.0029 (7)	−0.0026 (7)	0.0020 (7)
C5	0.0418 (8)	0.0438 (9)	0.0370 (9)	0.0036 (7)	−0.0019 (7)	−0.0044 (7)
C6	0.0386 (8)	0.0451 (9)	0.0388 (9)	0.0049 (7)	−0.0033 (7)	−0.0070 (7)
C6'	0.0470 (8)	0.0366 (8)	0.0383 (9)	−0.0011 (7)	−0.0075 (7)	0.0022 (7)
C7	0.0473 (9)	0.0451 (9)	0.0396 (9)	−0.0006 (7)	−0.0032 (7)	0.0011 (7)
O2	0.0637 (7)	0.0443 (7)	0.0494 (7)	0.0036 (5)	−0.0145 (6)	−0.0006 (5)
O3	0.0738 (9)	0.0588 (8)	0.0552 (8)	−0.0089 (6)	−0.0301 (7)	0.0021 (6)
O4	0.1656 (19)	0.0644 (11)	0.0883 (14)	−0.0240 (11)	−0.0110 (14)	−0.0248 (9)
O5	0.1369 (16)	0.0435 (9)	0.1173 (15)	−0.0002 (10)	0.0165 (13)	0.0075 (9)
O6	0.1006 (12)	0.0851 (11)	0.0517 (9)	0.0199 (9)	−0.0167 (8)	0.0157 (8)
O7	0.0696 (8)	0.0749 (10)	0.0509 (8)	0.0031 (7)	−0.0127 (7)	−0.0091 (7)
N7	0.0960 (14)	0.0448 (10)	0.0698 (13)	−0.0107 (9)	0.0257 (11)	−0.0044 (9)
N8	0.0529 (8)	0.0671 (11)	0.0386 (8)	0.0062 (8)	−0.0020 (7)	0.0070 (8)
C8	0.0385 (8)	0.0441 (9)	0.0413 (9)	−0.0038 (6)	−0.0006 (7)	0.0001 (7)
C9	0.0515 (9)	0.0498 (10)	0.0418 (10)	−0.0084 (8)	0.0003 (7)	−0.0041 (8)
C10	0.0583 (10)	0.0415 (10)	0.0508 (11)	−0.0045 (8)	0.0163 (8)	−0.0005 (8)
C11	0.0548 (10)	0.0484 (10)	0.0473 (10)	0.0065 (8)	0.0117 (8)	0.0102 (8)
C12	0.0427 (8)	0.0528 (10)	0.0365 (9)	0.0018 (7)	0.0026 (7)	0.0042 (7)
C13	0.0413 (8)	0.0429 (9)	0.0407 (9)	−0.0018 (7)	0.0004 (7)	0.0004 (7)
C14	0.0414 (8)	0.0485 (10)	0.0441 (10)	−0.0034 (7)	−0.0078 (7)	0.0032 (7)

Geometric parameters (Å, °)

O1—C4	1.235 (2)	N4'—H4B'	0.8602
O1'—C2'	1.2732 (19)	N6—H6A	0.8604
O2—C14	1.251 (2)	N6—H6B	0.8603
O3—C14	1.253 (2)	N6'—H6B'	0.8595
O4—N7	1.208 (3)	N6'—H6A'	0.8605
O5—N7	1.224 (3)	N7—C10	1.471 (3)
O6—N8	1.224 (2)	N8—C12	1.467 (2)
O7—N8	1.222 (2)	C1'—C6'	1.403 (2)

N1—C2	1.337 (2)	C1'—C7	1.514 (2)
N1—C6	1.388 (2)	C1'—C2'	1.391 (2)
N2—C2	1.317 (2)	C4—C5	1.420 (2)
N3—C4	1.405 (2)	C5—C7	1.518 (2)
N3—C2	1.329 (2)	C5—C6	1.375 (2)
N3'—C2'	1.384 (2)	C7—H7A	0.9696
N3'—C4'	1.357 (2)	C7—H7B	0.9701
N4'—C4'	1.331 (2)	C8—C9	1.392 (2)
N5'—C4'	1.320 (2)	C8—C13	1.386 (2)
N5'—C6'	1.369 (2)	C8—C14	1.517 (2)
N6—C6	1.342 (2)	C9—C10	1.384 (3)
N6'—C6'	1.337 (2)	C10—C11	1.376 (3)
N1—H1	0.8603	C11—C12	1.380 (3)
N2—H2B	0.8604	C12—C13	1.386 (2)
N2—H2A	0.8596	C9—H9	0.9295
N3—H3	0.8597	C11—H11	0.9293
N3'—H3'	0.8596	C13—H13	0.9302
N4'—H4A'	0.8608		
O1···N6'	2.929 (2)	C4···N7^{ii}	3.277 (3)
O1···N6^{i}	3.251 (2)	C4···N6'	3.335 (2)
O1···C10^{ii}	3.273 (2)	C4'···N3'^{xi}	3.426 (2)
O1'···N2^{iii}	2.991 (2)	C4'···C2'^{xi}	3.388 (2)
O1'···N3^{iii}	2.775 (2)	C5···N6'	3.379 (2)
O1'···C2^{iii}	3.302 (2)	C6'···O7^{i}	3.412 (2)
O1'···N6	2.916 (2)	C6'···O5^{iv}	3.355 (3)
O2···N1	2.663 (2)	C8···O2^{iv}	3.353 (2)
O2···C8^{iv}	3.353 (2)	C10···O1^{xvi}	3.273 (2)
O2···N8^{v}	3.049 (2)	C11···N1^{iv}	3.414 (2)
O2···C12^{v}	3.350 (2)	C12···N2^{iv}	3.449 (2)
O3···N2	2.781 (2)	C12···C2^{iv}	3.561 (2)
O3···O7^{v}	3.156 (2)	C12···O2^{v}	3.350 (2)
O3···N6'^{vi}	2.867 (2)	C13···C13^{v}	3.363 (2)
O3···N4'^{vii}	3.136 (2)	C14···N1	3.399 (2)
O4···O6^{viii}	3.096 (3)	C14···N8^{v}	3.284 (2)
O5···C1'^{iv}	3.419 (3)	C14···O7^{v}	2.995 (2)
O5···C6'^{iv}	3.355 (3)	C1'···H6A	2.9849
O5···C2'^{iv}	3.418 (3)	C2'···H2B^{iii}	3.0245
O6···O4^{ix}	3.096 (3)	C2'···H6A	2.7423
O6···N3'^{x}	3.056 (2)	C4···H6B'	2.6116
O7···C14^{v}	2.995 (2)	C4'···H4A'^{xiv}	3.0026
O7···O3^{v}	3.156 (2)	C5···H6B'	2.8598
O7···C6'^{iii}	3.412 (2)	C7···H6B'	2.5576
O7···N6'^{iii}	3.244 (2)	C7···H6A	2.6212

O1···H6B^{i}	2.6596	C9···H7A^{xvi}	3.0638
O1···H6B'	2.0883	C13···H13^{v}	3.0960
O1···H7A	2.5511	C14···H1	2.5868
O1'···H7B	2.5544	C14···H2A	2.7910
O1'···H3^{iii}	1.9719	H1···C14	2.5868
O1'···H6A	2.1038	H1···H2A	2.3013
O1'···H2B^{iii}	2.2714	H1···O2	1.8075
O2···H1	1.8075	H1···O3	2.7984
O2···H6B	2.6676	H1···H6B	2.2161
O2···H13	2.4896	H6A'···O3^{xv}	2.0570
O3···H2A	1.9469	H6A'···H2A^{xv}	2.4809
O3···H9	2.5078	H6B'···C7	2.5576
O3···H4B'^{vii}	2.5266	H6B'···H7A	2.2161
O3···H6A'^{vi}	2.0570	H6B'···C5	2.8598
O3···H1	2.7984	H6B'···O1	2.0883
O4···H9	2.4341	H6B'···C4	2.6116
O5···H11	2.4218	H2A···O3	1.9469
O6···H3'^{x}	2.3427	H2A···H6A'^{vi}	2.4809
O6···H11	2.4219	H2A···C14	2.7910
O7···H4B'^{x}	2.5594	H2A···H1	2.3013
O7···H3'^{x}	2.5430	H2B···C2'^{i}	3.0245
O7···H13	2.4439	H2B···H3	2.2679
O7···H7A^{iii}	2.8706	H2B···N5'^{vi}	2.8046
N1···C14	3.399 (2)	H2B···O1'^{i}	2.2714
N1···C11^{iv}	3.414 (2)	H2B···H3'^{i}	2.5706
N1···O2	2.663 (2)	H3···H2B	2.2679
N2···N8^{iv}	3.164 (2)	H3···O1'^{i}	1.9719
N2···C12^{iv}	3.449 (2)	H3···H6A^{i}	2.5774
N2···O3	2.781 (2)	H3'···O7^{xii}	2.5430
N2···N4'^{vii}	3.210 (2)	H3'···N8^{xii}	2.7093
N2···O1'^{i}	2.991 (2)	H3'···O6^{xii}	2.3427
N3···O1'^{i}	2.775 (2)	H3'···H4B'	2.2328
N3'···C4'^{xi}	3.426 (2)	H3'···H2B^{iii}	2.5706
N3'···O6^{xii}	3.056 (2)	H4A'···N5'^{xiv}	2.2305
N4'···O3^{xiii}	3.136 (2)	H4A'···C4'^{xiv}	3.0026
N4'···C2'^{xi}	3.363 (2)	H4A'···H4A'^{xiv}	2.4972
N4'···N5'^{xiv}	3.071 (2)	H4B'···O7^{xii}	2.5594
N4'···N2^{xiii}	3.210 (2)	H4B'···O3^{xiii}	2.5266
N5'···N4'^{xiv}	3.071 (2)	H4B'···H3'	2.2328
N6···O1^{iii}	3.251 (2)	H6A···H3^{iii}	2.5774
N6···C2'	3.409 (2)	H6A···C1'	2.9849
N6···O1'	2.916 (2)	H6A···C2'	2.7423
N6'···O1	2.929 (2)	H6A···O1'	2.1038

N6'···O7^{i}	3.244 (2)	H6A···H7B	2.2318
N6'···O3^{xv}	2.867 (2)	H6A···C7	2.6212
N6'···C4	3.335 (2)	H6B···O2	2.6676
N6'···C5	3.379 (2)	H6B···O1^{iii}	2.6596
N7···C4^{xvi}	3.277 (3)	H6B···H1	2.2161
N8···N2^{iv}	3.164 (2)	H7A···O1	2.5511
N8···C14^{v}	3.284 (2)	H7A···N6'	2.6903
N8···O2^{v}	3.049 (2)	H7A···H6B'	2.2161
N5'···H4A'^{xiv}	2.2305	H7A···C9^{ii}	3.0638
N5'···H2B^{xv}	2.8046	H7A···O7^{i}	2.8706
N6···H7B	2.6996	H7B···O1'	2.5544
N6'···H7A	2.6903	H7B···N6	2.6996
N8···H3'^{x}	2.7093	H7B···H6A	2.2318
C1'···O5^{iv}	3.419 (3)	H9···O3	2.5078
C2···O1'^{i}	3.302 (2)	H9···O4	2.4341
C2···C12^{iv}	3.561 (2)	H11···O5	2.4218
C2'···C4'^{xi}	3.388 (2)	H11···O6	2.4219
C2'···N6	3.409 (2)	H13···O2	2.4896
C2'···O5^{iv}	3.418 (3)	H13···O7	2.4439
C2'···N4'^{xi}	3.363 (2)	H13···C13^{v}	3.0960
C2—N1—C6	121.02 (14)	N4'—C4'—N5'	120.48 (14)
C2—N3—C4	124.17 (14)	N3'—C4'—N5'	122.19 (15)
C2'—N3'—C4'	123.12 (14)	N3'—C4'—N4'	117.32 (15)
C4'—N5'—C6'	116.65 (14)	C4—C5—C7	119.63 (14)
C2—N1—H1	119.47	C4—C5—C6	119.18 (15)
C6—N1—H1	119.50	C6—C5—C7	121.15 (14)
C2—N2—H2A	119.93	N6—C6—C5	124.66 (15)
H2A—N2—H2B	120.13	N1—C6—C5	120.48 (15)
C2—N2—H2B	119.95	N1—C6—N6	114.86 (14)
C2—N3—H3	117.92	N6'—C6'—C1'	121.19 (15)
C4—N3—H3	117.92	N5'—C6'—C1'	123.71 (15)
C4'—N3'—H3'	118.43	N5'—C6'—N6'	115.08 (14)
C2'—N3'—H3'	118.44	C1'—C7—C5	115.92 (13)
H4A'—N4'—H4B'	120.04	H7A—C7—H7B	107.40
C4'—N4'—H4A'	119.96	C1'—C7—H7A	108.33
C4'—N4'—H4B'	120.01	C1'—C7—H7B	108.29
H6A—N6—H6B	120.05	C5—C7—H7A	108.33
C6—N6—H6A	119.94	C5—C7—H7B	108.28
C6—N6—H6B	120.01	C9—C8—C13	119.86 (15)
C6'—N6'—H6A'	120.02	C9—C8—C14	120.44 (15)
H6A'—N6'—H6B'	119.91	C13—C8—C14	119.69 (15)
C6'—N6'—H6B'	120.07	C8—C9—C10	119.04 (16)
O4—N7—O5	124.3 (2)	N7—C10—C9	118.85 (17)
O4—N7—C10	118.20 (18)	N7—C10—C11	118.46 (17)
O5—N7—C10	117.50 (19)	C9—C10—C11	122.68 (17)

O6—N8—C12	118.25 (17)	C10—C11—C12	116.73 (16)
O7—N8—C12	118.97 (16)	N8—C12—C11	118.24 (15)
O6—N8—O7	122.78 (16)	N8—C12—C13	118.79 (16)
C6'—C1'—C7	121.73 (14)	C11—C12—C13	122.97 (15)
C2'—C1'—C6'	117.81 (14)	C8—C13—C12	118.70 (16)
C2'—C1'—C7	120.46 (14)	O2—C14—O3	125.66 (17)
N1—C2—N2	120.42 (15)	O2—C14—C8	117.35 (15)
N1—C2—N3	119.24 (15)	O3—C14—C8	116.97 (16)
N2—C2—N3	120.31 (15)	C8—C9—H9	120.39
N3'—C2'—C1'	116.21 (14)	C10—C9—H9	120.57
O1'—C2'—C1'	126.22 (15)	C10—C11—H11	121.69
O1'—C2'—N3'	117.57 (14)	C12—C11—H11	121.58
N3—C4—C5	115.76 (15)	C8—C13—H13	120.66
O1—C4—N3	117.41 (15)	C12—C13—H13	120.64
O1—C4—C5	126.83 (16)		
C6—N1—C2—N2	179.24 (15)	C2'—C1'—C6'—N5'	−6.9 (2)
C6—N1—C2—N3	1.1 (2)	C2'—C1'—C6'—N6'	174.52 (15)
C2—N1—C6—N6	−178.93 (14)	C7—C1'—C6'—N6'	−5.3 (2)
C2—N1—C6—C5	1.7 (2)	C2'—C1'—C7—C5	−100.30 (17)
C4—N3—C2—N1	−4.2 (2)	O1—C4—C5—C7	0.8 (2)
C4—N3—C2—N2	177.67 (15)	N3—C4—C5—C6	−1.2 (2)
C2—N3—C4—O1	−175.53 (15)	O1—C4—C5—C6	178.47 (16)
C2—N3—C4—C5	4.2 (2)	N3—C4—C5—C7	−178.87 (13)
C4'—N3'—C2'—O1'	−179.83 (14)	C6—C5—C7—C1'	80.93 (18)
C4'—N3'—C2'—C1'	−0.4 (2)	C7—C5—C6—N6	−3.2 (2)
C2'—N3'—C4'—N4'	177.70 (15)	C4—C5—C7—C1'	−101.45 (17)
C2'—N3'—C4'—N5'	−1.3 (2)	C4—C5—C6—N1	−1.5 (2)
C6'—N5'—C4'—N3'	−1.0 (2)	C4—C5—C6—N6	179.18 (15)
C6'—N5'—C4'—N4'	−180.00 (15)	C7—C5—C6—N1	176.09 (14)
C4'—N5'—C6'—N6'	−176.13 (15)	C13—C8—C9—C10	0.7 (2)
C4'—N5'—C6'—C1'	5.2 (2)	C14—C8—C9—C10	−178.25 (14)
O4—N7—C10—C9	6.2 (3)	C9—C8—C13—C12	−1.3 (2)
O4—N7—C10—C11	−175.0 (2)	C14—C8—C13—C12	177.66 (14)
O5—N7—C10—C9	−172.20 (19)	C9—C8—C14—O2	−176.92 (15)
O5—N7—C10—C11	6.5 (3)	C9—C8—C14—O3	4.6 (2)
O6—N8—C12—C11	0.3 (2)	C13—C8—C14—O2	4.1 (2)
O7—N8—C12—C11	−179.76 (15)	C13—C8—C14—O3	−174.33 (15)
O6—N8—C12—C13	−178.79 (15)	C8—C9—C10—N7	179.28 (16)
O7—N8—C12—C13	1.1 (2)	C8—C9—C10—C11	0.6 (2)
C7—C1'—C2'—N3'	−175.99 (14)	N7—C10—C11—C12	−179.93 (17)
C6'—C1'—C2'—O1'	−176.43 (15)	C9—C10—C11—C12	−1.2 (2)
C7—C1'—C2'—O1'	3.4 (2)	C10—C11—C12—N8	−178.47 (14)
C6'—C1'—C2'—N3'	4.2 (2)	C10—C11—C12—C13	0.6 (2)
C6'—C1'—C7—C5	79.49 (19)	N8—C12—C13—C8	179.72 (14)
C7—C1'—C6'—N5'	173.27 (15)	C11—C12—C13—C8	0.7 (2)

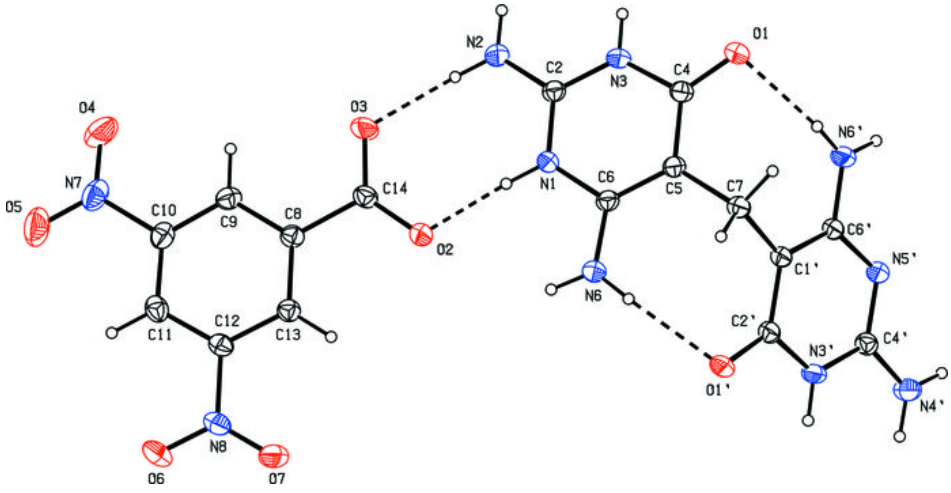
Symmetry codes: (i) *x*+1/2, −*y*+1/2, *z*+1/2; (ii) −*x*−1/2, *y*−1/2, −*z*+1/2; (iii) *x*−1/2, −*y*+1/2, *z*−1/2; (iv) −*x*, −*y*+1, −*z*; (v) −*x*−1, −*y*+1, −*z*; (vi) −*x*+1/2, *y*+1/2, −*z*+1/2; (vii) *x*−1/2, −*y*+1/2, *z*+1/2; (viii) *x*+1/2, −*y*+3/2, *z*+1/2; (ix) *x*−1/2, −*y*+3/2, *z*−1/2; (x) −*x*−1/2, *y*+1/2, −*z*−1/2; (xi) −*x*, −*y*, −*z*; (xii) −*x*−1/2, *y*−1/2, −*z*−1/2; (xiii) *x*+1/2, −*y*+1/2, *z*−1/2; (xiv) −*x*+1, −*y*, −*z*; (xv) −*x*+1/2, *y*−1/2, −*z*+1/2; (xvi) −*x*−1/2, *y*+1/2, −*z*+1/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O2	0.86	1.81	2.663 (2)	173
N6'—H6A'···O3^{xv}	0.86	2.06	2.867 (2)	156
N6'—H6B'···O1	0.86	2.09	2.929 (2)	166
N2—H2A···O3	0.86	1.95	2.781 (2)	163
N2—H2B···O1'^{i}	0.86	2.27	2.991 (2)	141
N3—H3···O1'^{i}	0.86	1.97	2.775 (2)	155
N3'—H3'···O6^{xii}	0.86	2.34	3.056 (2)	141
N4'—H4A'···N5'^{xiv}	0.86	2.23	3.071 (2)	165
N4'—H4B'···O7^{xii}	0.86	2.56	3.355 (2)	154
N4'—H4B'···O3^{xiii}	0.86	2.53	3.136 (2)	129
N6—H6A···O1'	0.86	2.10	2.916 (2)	157
C7—H7A···O1	0.97	2.55	2.930 (2)	103
C7—H7B···O1'	0.97	2.55	2.925 (2)	103

Symmetry codes: (xv) −*x*+1/2, *y*−1/2, −*z*+1/2; (i) *x*+1/2, −*y*+1/2, *z*+1/2; (xii) −*x*−1/2, *y*−1/2, −*z*−1/2; (xiv) −*x*+1, −*y*, −*z*; (xiii) *x*+1/2, −*y*+1/2, *z*−1/2.

Fig. 1


O4
O3
N2
C2
N3
C4
O1
N6'
N7
C14
N1
C6
C5
C7
O5
C10
C9
C8
O2
C6'
C1'
N5'
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C11
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C13
N3'
O1'
N4'
N8
O6
O7

Fig. 2

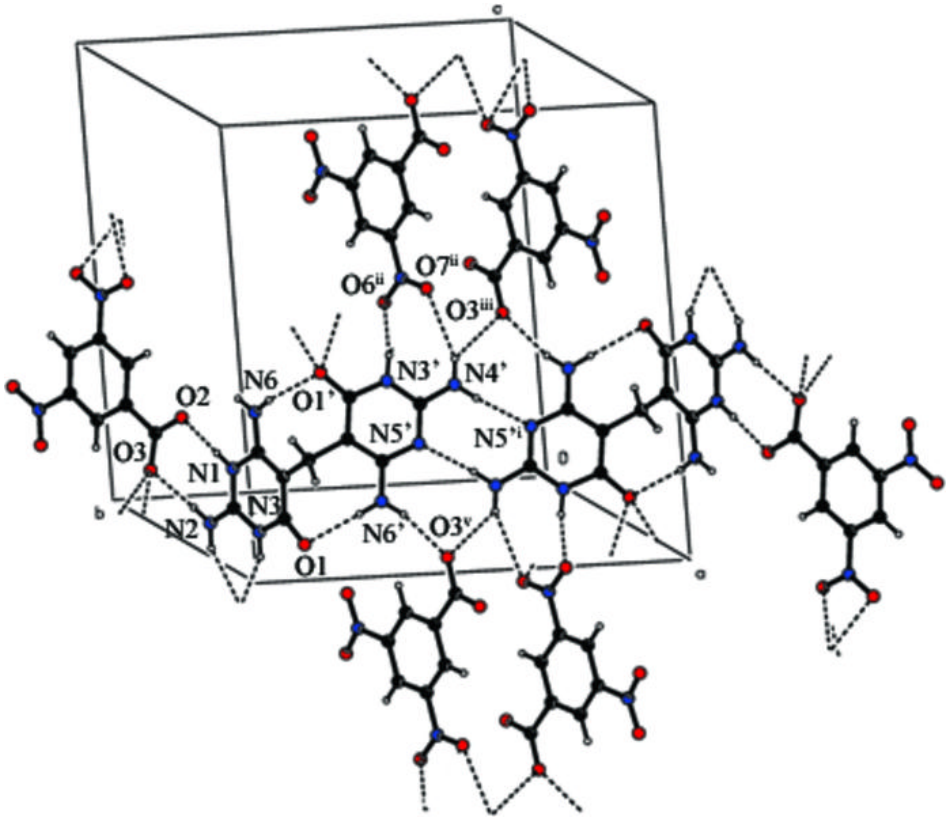

Fig. 3