Crystal structure and Hirshfeld surface analysis of 2,4,6-triaminopyrimidin-1,3-diium dinitrate

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The title compound, C₆H₉N₅²⁺·2NO₃⁻, crystallizes in the monoclinic crystal system, space group P2₁/c. The asymmetric unit, which comprises a diprotonated triaminopyrimidine dication and two nitrate anions, has an almost planar geometry with a dihedral angle of 0.92 (4)° between the mean plane of the cation and that defined by both anions. In the crystal, hydrogen-bonding interactions between the 2,4,6-triaminopyrimidine cation and the nitrate anions lead to a one-dimensional supramolecular network with weak anionic interactions forming a three-dimensional network. These interactions were investigated using Hirshfeld surface analysis, which indicates that the most important contributions for the packing arrangement are from O···H/H···O (53.2%), N···H/H···N (12.5%) and C···H/H···C (9.6%) interactions. Energy framework analysis showed that of the components of the framework energies, electrostatic repulsion (E_{rep}) is dominant.

1. Chemical context

Nitrogen heterocycles and pyrimidines are examples of the most important biologically active compounds and find wide use in modern medicine (Palasz & Ciezà, 2015; Takeshita et al., 2006; Henderson et al., 2003). Pyrimidine derivatives are used as intermediates for the production of various complex organic molecules for the treatment of cancer and AIDS (Fawcett et al., 1996). Several pyrimidine derivatives belong to the class of central nervous system depressants (Soayed et al., 2015). Pyrimidine and its derivatives have great importance as they constitute a significant class of natural and non-natural products, many of which possess remarkable biological activities and clinical applications such as antibacterial, antimalarial and anticancer agents (Sharma et al., 2014). Many pyrimidine derivatives are reported to possess potential central nervous system (CNS) depressant properties and also act as calcium channel blockers (Kumar et al., 2002). Pyrimido[4,5-d]pyrimidine-2,5-dione and 2,4-diamino-5-(substituted)pyrimidines have been reported to have potent antimicrobial activity (Sharma et al., 2004) and 2,4,6-triaminopyrimidine (TAP) acts as a fast-killing and long-acting antimalarial agent (Hameed, et al., 2015). It is also known to inhibit sodium transport in the skin of frogs (Bowman et al., 1978). It can be synthesized by a regioselective cycloaddition process in high yield by reaction between two moles of...
cyanamide and one mole of ynamide in the presence of triflic acid as catalyst (Dubovtsev, et al., 2021). Many pyrimidine derivatives display interesting optical and sensing properties (Achelle et al., 2012; Seenan et al., 2020). Methylpyrimidinium push–pull derivatives have been shown to be promising materials for optical data processing. Organometallic methylpyrimidinium chromophores incorporating a ruthenium fragment within the π-conjugated spacer are among the best metal–diyne NLO chromophores (Fecková et al., 2020). Herein, we report the structure of 2,4,6-triamino-1,3,5-triazine-1,3-dium dinitrate, Fig. 1, which was synthesized via reaction of 2,4,6-triaminopyrimidine with nitric acid.

![Image](https://example.com/image1.png)

**Figure 1**

**ORTEP** diagram of the title compound with atom labeling and 50% probability ellipsoids.

2. Structural commentary

In the asymmetric unit, the mean planes of the nitrate anions are inclined to one another by 5.97°. The plane of the anion containing N6 is inclined to the mean plane of the cation by 3.25° while that of the other anion is inclined by 2.84°. Thus the whole asymmetric unit lies close to a common plane (Fig.1). The ring C—N bond lengths in the cation [C1—N2 = 1.3531 (16) Å and C2—N3 = 1.3267 (16) Å] are only slightly altered from those in the corresponding conjugate base (Schwalbe et al., 1982). The C—C bond lengths in the pyrimidine ring [C2—C3 = 1.3834 (18) Å and C3—C4 = 1.3888 (17) Å] are consistent with literature values (Ali et al., 2021). The exocyclic C2—N3 and C4—N4 bond lengths [1.3267 (16) Å and 1.3240 (17) Å, respectively] are equivalent within experimental error but the C1—N1 bond length is markedly shorter at 1.3010 (17) Å. As it lies between the two protonated ring nitrogen atoms, this suggests that the neighboring positive charge induces a contribution from a charge-separated quinoid form to the overall electronic structure, as has been proposed for the analogous chloride salt (Portalone & Colapietro, 2007).

3. Supramolecular features

In the crystal, a combination of N1—H1A···O2, N5—H5···O4, N4—H4A···O6, N3—H1A···O3 and N3—H3B···O5 hydrogen bonds (Table 1) leads to the formation of ribbons of alternating cations and anions extending along the b-axis direction. The mean planes of the ribbons are parallel to (101). Pairs of adjacent ribbons are linked by N1—H1B···O3, N2—H2···O1 and N3—H3A···O3 hydrogen bonds (Table 1), with these units further connected into cation/anion layers by complementary N4—H4B···O6 hydrogen bonds. The two unique nitrate ions are connected to the cation by N—H···O hydrogen bonds (Table 1), forming units with an $R_2^2(8)$ graph-set motif (Fig. 2). This tight hydrogen-bonded network causes a short O2···O4 contact of 2.7752 (15) Å. Finally, the layers appear to be associated through N=N=O···π(ring) interactions N6=O3···Cg1 and N7=O5···Cg1 (Cg1 is the centroid of the pyrimidine ring at $-x + 1, -y + 1, -z + 1$; Cg is the

![Image](https://example.com/image2.png)

**Figure 2**

A portion of one cation/anion layer projected onto (101) with N—H···O hydrogen bonds depicted by dashed lines.

**Table 1**

| Hydrogen-bond geometry (Å, °) | $D$—H···$A$ | $D$—H···$A$ | $D$—H···$A$ | $D$—H···$A$ |
|-----------------------------|------------|------------|------------|------------|
| N5—H5···O4                 | 0.86       | 1.88       | 2.7321 (15) | 174        |
| N2—H2···O1                 | 0.86       | 1.98       | 2.8319 (15) | 169        |
| N4—H4A···O6                | 0.86       | 2.08       | 2.9428 (15) | 177        |
| N4—H4B···O5               | 0.86       | 2.43       | 3.0706 (16) | 131        |
| N4—H4B···O6               | 0.86       | 2.11       | 2.9593 (15) | 172        |
| N1—H1A···O2               | 0.86       | 1.97       | 2.7966 (15) | 160        |
| N1—H1B···O3              | 0.86       | 1.94       | 2.7912 (15) | 172        |
| N3—H3A···O3            | 0.86       | 2.16       | 3.0018 (14) | 167        |
| N3—H3A···O2          | 0.86       | 2.54       | 2.9770 (15) | 113        |
| N3—H3B···O5       | 0.86       | 2.26       | 3.0619 (15) | 156        |
| C3—H3···O5          | 0.93       | 2.56       | 3.3134 (16) | 139        |

Symmetry codes: (i) $-x + 1, -y + 1, -z + 1$; (ii) $-x + 2, y, -z + 1/2$; (iii) $x, y, 1$. 

**References**

Dubovtsev, et al., 2021; Seenan et al., 2020; Ali et al., 2021; Schwalbe et al., 1982; Portalone & Colapietro, 2007.
4. Hirshfeld Surface Analysis

The Hirshfeld surface analysis (Spackman & Jayatilaka et al., 2009) was performed and the two-dimensional fingerprint plots (McKinnon et al., 2007) were generated with Crystal Explorer17 (Turner et al., 2017) to quantify the intermolecular contacts present within the crystal structure. The Hirshfeld surface is mapped over \( d_{\text{norm}} \) in the range \(-0.6823\) to \(0.9826\) in arbitrary units with colors ranging from red (shorter distance than the sum of van der Waals radii) through white to blue (longer distance than the sum of the van der Waals radii). Top and bottom views of the surface together with curvedness, and shape-index plots are given in Fig. 4a–d. The red spots symbolize N–H⋯O contacts and C–H⋯O interactions. The fingerprint plots (Fig. 5) give an insight into the overall packing characteristics of the contents of the unit cell, being plots of \( d_e \) versus \( d_i \), where \( d_i \) is the distance to the nearest atom center interior to the surface, and \( d_e \) to the nearest atom exterior to the surface. These plots show that the main contributions to the overall surface involve O⋯H/H⋯O contacts at 53.2% (Fig. 5b), followed by N⋯H/H⋯N contacts at 12.5% (Fig. 5c) and C⋯H/H⋯C contacts at 9.6% (Fig. 5d).

5. Synthesis and crystallization

To synthesize the title compound, 20 mg of 2,4,6-triamino-pyrimidine were dissolved in ethanol (10 mL) and the solution stirred for 3 h. A mixture of ethanol (5 mL) and nitric acid (0.5 mL) was taken in a separate round-bottom flask and stirred for 3 h at 333 K. Afterwards, the 2,4,6-triamino-
pyrimidine solution was added dropwise to the above mixture. The reaction was continued for 4 h at the same temperature. After completion of the reaction, a pale-yellow solution was obtained, which was filtered and kept for slow evaporation at room temperature. After 15 days, pale-yellow crystals were obtained that were suitable for data collection (Fig. 6).

6. Interaction energy calculations

The interaction energies for the title compound (Fig. 7) were computed using the HF/3-21G quantum level of theory, which is available in CrystalExplorer 17.5. Electrostatic ($E_{\text{ele}}$), polarization ($E_{\text{pol}}$), dispersion ($E_{\text{disp}}$), and exchange-repulsion ($E_{\text{rep}}$) are the four energy variables that make up the total intermolecular interaction energy ($E_{\text{tot}}$). Cylinder-shaped energy frameworks represent the relative strengths of interaction energies in individual directions and give the topologies of pair-wise intermolecular interaction energies within the crystal (Mackenzie et al., 2017). The energies between molecular pairs are represented as cylinders connecting the centroids of pairs of molecules, with the cylinder radius equal to the amount of interaction energy between the molecules (Wu et al., 2020). The dark-blue-colored molecule at symmetry position ($x, -y + \frac{1}{2}, z + \frac{1}{2}$) located 6.25 Å from the centroid of the selected molecule has the highest total interaction energy of $-40.1 \text{kJ mol}^{-1}$, as shown in Fig. 7. The net interaction energies for the title compound are $E_{\text{ele}} = -58.9 \text{kJ mol}^{-1}$, $E_{\text{pol}} = -92.0 \text{kJ mol}^{-1}$, $E_{\text{disp}} = -148.8 \text{kJ mol}^{-1}$, $E_{\text{rep}} = 176.9 \text{kJ mol}^{-1}$, with a total interaction energy $E_{\text{tot}}$ of $-110.4 \text{kJ mol}^{-1}$ (Fig. 8). Clearly, $E_{\text{rep}}$ is the major interaction energy in the title compound.
Table 2
Experimental details.

| Crystal data | Chemical formula | C₂H₇N₄²⁺·2NO₃⁻ |
|--------------|------------------|-----------------|
| M₁           | 251.18           |                 |
| Crystal system, space group | Monoclinic, P2₁/c  |
| Temperature (K) | 276              |
| a, b, c (Å)   | 7.8650 (5), 9.9173 (6), 12.2291 (7) |
| β (°)        | 100.856 (2)      |
| V (Å³)       | 936.86 (10)      |
| Z            | 4                |
| Radiation type | Mo Kα            |
| Crystal size (mm) | 0.37 × 0.27 × 0.14 |

Data collection

| Diffractometer | Bruker APEXII CCD |
|----------------|-------------------|
| No. of measured, independent and observed [I > 2σ(I)] reflections | 13469, 2312, 1993 |
| R(1/λ)max (Å⁻¹) | 0.070 |
| S               | 0.040, 0.110, 1.07 |
| No. of reflections | 2312 |
| No. of parameters | 154 |
| H-atom treatment | H-atom parameters constrained |
| Δρmax, Δρmin (e Å⁻³) | 0.51, –0.30 |

Refinement

| R(F² > 2σ(F²)), wR(F²), S | 0.040, 0.110, 1.07 |
| No. of reflections | 2312 |
| No. of parameters | 154 |
| H-atom treatment | H-atom parameters constrained |
| Δρmax, Δρmin (e Å⁻³) | 0.51, –0.30 |

Computer programs: X-AREA and X-RED32 (Stoe & Cie, 2002), SHELXT2018/3 (Sheldrick, 2015a), SHELXL2018/3 (Sheldrick, 2015b), OLEX2 (Dolomanov et al., 2009), Mercury (Macrae et al., 2020), WinGX (Farrugia, 2012), PLATON (Spek, 2009) and pubICIF (Westrip, 2010).

7. Database survey

A search of the Cambridge Structural Database (CSD, Version 5.43, update of March 2022; Groom et al., 2016) for the triaminopyrimidine dication gave 24 hits of which 16 were for the FPO₂⁻ salt studied at a variety of temperatures (GESWAF–GESWAF15; Matulková et al., 2017) but no structure containing nitrate anions was found. The remaining structures contain arenosulfonate (TEYTEZ, TEYTID and TEYXIIH; Karak et al., 2018), various polycarboxylate (VEXQEX, VEXZW and VEBEJ; Xing et al., 2017), chloride (GIMROK; Portalone & Colapietro, 2007) and [Cu₃Cl₈]²⁺ (GOHDYO; Voronina et al., 2012) anions. Most of the discussions of these structures are concerned more with their supramolecular details than the detailed geometry of the cation but, as noted in Section 3, some details similar to those in the present work are seen in the structure of the chloride salt.

8. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. All H atoms were originally found in difference maps. They were positioned geometrically (N–H = 0.86 Å, C–H = 0.93 Å) and refined as riding with Uiso(H) = 1.2Ueq(C,N).

Acknowledgements

The authors are grateful to the Department of Applied Chemistry, Aligarh Muslim University, for providing laboratory facilities. Author contributions are as follows. Conceptualization, SD and EB; methodology, AimanA and ArifA; investigation, SD and AdeebaA; writing (original draft), SD, EB; and ND; writing (review and editing of the manuscript), AlmA and ArifA; visualization, MA and AJA; supervision, ES and ND.

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Computing details

Data collection: X-AREA (Stoe & Cie, 2002); cell refinement: X-AREA (Stoe & Cie, 2002); data reduction: X-RED32 (Stoe & Cie, 2002); program(s) used to solve structure: SHELXT2018/3 (Sheldrick, 2015a); program(s) used to refine structure: SHELXL2018/3 (Sheldrick, 2015b); molecular graphics: OLEX2 (Dolomanov et al., 2009) and Mercury (Macrae et al., 2020); software used to prepare material for publication: WinGX (Farrugia, 2012), SHELXL2018/3 (Sheldrick, 2015b), PLATON (Spek, 2020) and publCIF (Westrip, 2010).

2,4,6-Triaminopyrimidine-1,3-diium dinitrate

Crystal data

C4H9N52+·2NO3−

Mr = 251.18

Monoclinic, P21/c

a = 7.8650 (5) Å

b = 9.9173 (6) Å

c = 12.2291 (7) Å

β = 100.836 (2)°

V = 936.86 (10) Å3

Z = 4

F(000) = 520

Dx = 1.781 Mg m−3

Mo Kα radiation, λ = 0.71073 Å

Cell parameters from 8448 reflections

θ = 2.3–25.6°

µ = 0.16 mm−1

T = 276 K

Needle, colourless

0.37 × 0.27 × 0.14 mm

Data collection

Bruker APEXII CCD
diffractometer

φ and ω scans

13469 measured reflections

2312 independent reflections

1993 reflections with I > 2σ(I)

Refinement

Refinement on F2

Least-squares matrix: full

R[F2 > 2σ(F2)] = 0.040

wR(F2) = 0.110

S = 1.07

2312 reflections

154 parameters

0 restraints

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

w = 1/[σ2(Fo2) + (0.0497P)2 + 0.4576P]

where P = (Fo2 + 2Fc2)/3

(Δ/σ)max < 0.001

Δρmax = 0.51 e Å−3

Δρmin = −0.30 e Å−3
Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

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

|    | x     | y     | z     | U(eq)  |
|----|-------|-------|-------|--------|
| O3 | 0.54263 (12) | 0.80420 (9) | 0.71416 (8) | 0.0141 (2) |
| O5 | 0.88490 (13) | 0.76472 (9) | 0.36706 (8) | 0.0148 (2) |
| O1 | 0.50750 (13) | 0.59279 (10) | 0.75438 (8) | 0.0168 (2) |
| O6 | 0.93192 (13) | 0.56691 (10) | 0.30278 (8) | 0.0173 (2) |
| O4 | 0.80491 (14) | 0.58662 (10) | 0.44532 (8) | 0.0207 (2) |
| O2 | 0.64974 (14) | 0.64786 (10) | 0.62512 (9) | 0.0205 (2) |
| N5 | 0.77821 (13) | 0.31443 (11) | 0.47214 (9) | 0.0099 (2) |
| H5 | 0.787384 | 0.398958 | 0.458958 | 0.012* |
| N2 | 0.68341 (13) | 0.14353 (11) | 0.57534 (9) | 0.0105 (2) |
| H2 | 0.634287 | 0.118719 | 0.629218 | 0.013* |
| N4 | 0.92308 (15) | 0.27225 (11) | 0.32949 (9) | 0.0128 (2) |
| H4A | 0.929637 | 0.358122 | 0.321423 | 0.015* |
| H4B | 0.967123 | 0.218902 | 0.286854 | 0.015* |
| N6 | 0.56691 (14) | 0.68070 (11) | 0.69851 (9) | 0.0115 (2) |
| N7 | 0.87310 (14) | 0.63926 (11) | 0.37153 (9) | 0.0116 (2) |
| N1 | 0.63901 (14) | 0.36592 (11) | 0.61695 (9) | 0.0130 (2) |
| H1A | 0.649848 | 0.450490 | 0.604304 | 0.016* |
| H1B | 0.588658 | 0.340225 | 0.670025 | 0.016* |
| N3 | 0.71841 (14) | −0.08175 (11) | 0.53700 (9) | 0.0131 (2) |
| H3A | 0.666228 | −0.100504 | 0.590919 | 0.016* |
| H3B | 0.754039 | −0.145693 | 0.499473 | 0.016* |
| C1 | 0.69879 (15) | 0.27685 (13) | 0.55581 (10) | 0.0103 (3) |
| C4 | 0.84517 (15) | 0.22217 (13) | 0.40753 (10) | 0.0101 (3) |
| C3 | 0.82632 (16) | 0.08538 (12) | 0.42648 (10) | 0.0103 (3) |
| H3 | 0.868341 | 0.021484 | 0.382632 | 0.012* |
| C2 | 0.74394 (15) | 0.04582 (13) | 0.51170 (10) | 0.0106 (2) |

Atomic displacement parameters (Å²)

|    | U¹¹  | U²²  | U³³  | U¹²  | U¹³  | U²³  |
|----|------|------|------|------|------|------|
| O3 | 0.0184 (5) | 0.0101 (4) | 0.0138 (5) | 0.0018 (3) | 0.0028 (4) | −0.0004 (3) |
| O5 | 0.0195 (5) | 0.0105 (5) | 0.0130 (5) | −0.0005 (4) | −0.0006 (4) | 0.0002 (3) |
| O1 | 0.0244 (5) | 0.0126 (5) | 0.0153 (5) | −0.0007 (4) | 0.0088 (4) | 0.0021 (3) |
| O6 | 0.0254 (5) | 0.0144 (5) | 0.0140 (5) | 0.0018 (4) | 0.0088 (4) | −0.0018 (4) |
| O4 | 0.0344 (6) | 0.0149 (5) | 0.0166 (5) | −0.0011 (4) | 0.0142 (4) | 0.0018 (4) |
| O2 | 0.0328 (6) | 0.0141 (5) | 0.0189 (5) | 0.0008 (4) | 0.0163 (4) | −0.0014 (4) |
| N5 | 0.0140 (5) | 0.0081 (5) | 0.0071 (5) | −0.0002 (4) | 0.0005 (4) | 0.0004 (4) |
| N2 | 0.0133 (5) | 0.0113 (5) | 0.0068 (5) | −0.0011 (4) | 0.0018 (4) | 0.0008 (4) |
| N4 | 0.0187 (5) | 0.0116 (5) | 0.0087 (5) | 0.0005 (4) | 0.0041 (4) | 0.0004 (4) |
Geometric parameters (Å, °)

\[
\begin{array}{cccc}
\text{O3—N6} & 1.2597 (14) & \text{N4—C4} & 1.3240 (17) \\
\text{O5—N7} & 1.2496 (14) & \text{N4—H4A} & 0.8600 \\
\text{O1—N6} & 1.2511 (15) & \text{N4—H4B} & 0.8600 \\
\text{O6—N7} & 1.2577 (15) & \text{N1—C1} & 1.3010 (17) \\
\text{O4—N7} & 1.2476 (15) & \text{N1—H1A} & 0.8600 \\
\text{O2—N6} & 1.2473 (15) & \text{N1—H1B} & 0.8600 \\
\text{N5—C1} & 1.3477 (16) & \text{N3—C2} & 1.3267 (16) \\
\text{N5—C4} & 1.3767 (16) & \text{N3—H3A} & 0.8600 \\
\text{N5—H5} & 0.8600 & \text{N3—H3B} & 0.8600 \\
\text{N2—C1} & 1.3531 (16) & \text{C4—C3} & 1.3888 (17) \\
\text{N2—C2} & 1.3822 (16) & \text{C3—C2} & 1.3834 (18) \\
\text{N2—H2} & 0.8600 & \text{C3—H3} & 0.9300 \\
\text{C1—N5—C4} & 122.26 (11) & \text{H1A—N1—H1B} & 120.0 \\
\text{C1—N5—H5} & 118.9 & \text{C2—N3—H3A} & 120.0 \\
\text{C4—N5—H5} & 118.9 & \text{C2—N3—H3B} & 120.0 \\
\text{C1—N2—C2} & 122.27 (11) & \text{N3—C2} & 120.0 \\
\text{C1—N2—H2} & 118.9 & \text{N3—N5—C1} & 121.18 (12) \\
\text{C2—N2—H2} & 118.9 & \text{N2—N5—C1} & 120.53 (12) \\
\text{C4—N4—H4A} & 120.0 & \text{N5—N2—C1} & 118.28 (11) \\
\text{C4—N4—H4B} & 120.0 & \text{N4—C4—N5} & 116.31 (11) \\
\text{H4A—N4—H4B} & 120.0 & \text{N4—C4—C3} & 124.41 (12) \\
\text{O2—N6—O1} & 120.68 (11) & \text{N5—C4—C3} & 119.28 (11) \\
\text{O2—N6—O3} & 118.54 (11) & \text{C2—C3—C4} & 118.85 (12) \\
\text{O1—N6—O3} & 120.78 (11) & \text{C2—C3—H3} & 120.6 \\
\text{O4—N7—O5} & 119.59 (11) & \text{C4—C3—H3} & 120.6 \\
\text{O4—N7—O6} & 120.46 (11) & \text{N3—C2—N2} & 117.00 (11) \\
\text{O5—N7—O6} & 119.94 (11) & \text{N3—C2—C3} & 123.98 (12) \\
\text{C1—N1—H1A} & 120.0 & \text{N2—C2—C3} & 119.02 (11) \\
\text{C1—N1—H1B} & 120.0 & \text{N4—C4—C3} & 179.23 (12) \\
\text{C4—N5—C1—N1} & 178.85 (11) & \text{N5—C4—C3} & 179.23 (12) \\
\text{C4—N5—C1—N2} & −0.76 (17) & \text{N5—C4—C3} & −1.46 (17) \\
\text{C2—N2—C1—N1} & 179.46 (11) & \text{C1—N2—C2—N3} & −178.59 (10) \\
\text{C2—N2—C1—N5} & −0.93 (17) & \text{C1—N2—C2—C3} & 1.36 (17) \\
\text{C1—N5—C4—N4} & −178.68 (11) & \text{C4—C3—C2—N3} & 179.81 (11) \\
\text{C1—N5—C4—C3} & 1.96 (17) & \text{C4—C3—C2—N2} & −0.13 (17)
\end{array}
\]
Hydrogen-bond geometry (Å, °)

| D—H···A     | D—H | H···A | D···A   | D—H···A |
|-------------|-----|-------|---------|---------|
| N5—H5···O4  | 0.86| 1.88  | 2.7321 (15) | 174     |
| N2—H2···O1i | 0.86| 1.98  | 2.8319 (15) | 169     |
| N4—H4A···O6 | 0.86| 2.08  | 2.9428 (15) | 177     |
| N4—H4B···O5ii | 0.86| 2.43  | 3.0706 (16) | 131     |
| N4—H4B···O6ii | 0.86| 2.11  | 2.9593 (15) | 172     |
| N4—H4B···N7ii | 0.86| 2.62  | 3.4400 (16) | 160     |
| N1—H1A···O2  | 0.86| 1.97  | 2.7986 (15) | 160     |
| N1—H1A···N6  | 0.86| 2.69  | 3.3577 (16) | 135     |
| N1—H1B···O3i | 0.86| 1.94  | 2.7912 (15) | 172     |
| N3—H3A···O3iii | 0.86| 2.16  | 3.0018 (14) | 167     |
| N3—H3A···O2iii | 0.86| 2.54  | 2.9770 (15) | 113     |
| N3—H3B···O5iii | 0.86| 2.26  | 3.0619 (15) | 156     |
| C3—H3···O5iii | 0.93| 2.56  | 3.3134 (16) | 139     |

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