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4-Nitrophenol–2,4,6-triamino-1,3,5-triazine–water (2/1/1)

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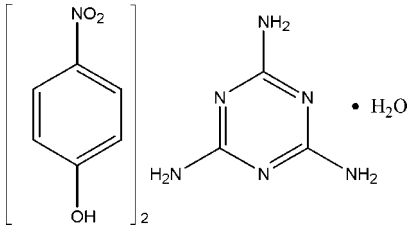
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.002 Å; R factor = 0.043; wR factor = 0.122; data-to-parameter ratio = 18.3.

In the title adduct, $2C_6H_5NO_3\cdot C_3H_6N_6\cdot H_2O$, the melamine and the two independent nitrophenol molecules are essentially planar, with maximum deviations of 0.0294 (10), 0.0706 (12) and 0.0742 (12) Å, respectively. In the crystal, N—H···N, O—H···N, N—H···O and O—H···O hydrogen bonds link the components into a three-dimensional network. In addition, weak π–π interactions [centroid–centroid distances = 3.728 (3) and 3.749 (3) Å] are observed.

Related literature

For applications of melamine, see: Cook *et al.* (2005); Rima *et al.* (2008). For a related structure, see: Cousson *et al.* (2005).



Experimental

Crystal data

$2C_6H_5NO_3\cdot C_3H_6N_6\cdot H_2O$
M_r = 422.37
Triclinic, $P\overline{1}$
a = 7.123 (5) Å
b = 10.577 (4) Å
c = 13.680 (5) Å
α = 68.256 (5)°
β = 88.772 (6)°
γ = 76.604 (5)°
V = 928.9 (8) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.12 mm^{-1}
T = 295 K
0.30 × 0.20 × 0.20 mm

Data collection

Bruker Kappa APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.964, T_{max} = 0.976
21610 measured reflections
5696 independent reflections
4164 reflections with $I > 2\sigma(I)$
R_{int} = 0.030

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.122
S = 1.03
5696 reflections
311 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O7^{i}	0.90 (2)	1.76 (2)	2.6600 (18)	172 (2)
O4—H4···N5	0.91 (2)	1.87 (2)	2.7217 (16)	157 (2)
O7—H7*A*···N4	0.88 (2)	1.94 (2)	2.8020 (18)	166 (2)
O7—H7*B*···O2^{iv}	0.84 (2)	2.22 (2)	3.0424 (18)	164 (2)
N6—H6*A*···O6^{ii}	0.860 (18)	2.363 (19)	3.0276 (16)	134 (2)
N6—H6*B*···N3^{iii}	0.845 (18)	2.235 (19)	3.080 (2)	178 (2)
N7—H7*C*···O6^{v}	0.867 (17)	2.250 (17)	3.056 (2)	155 (2)
N7—H7*D*···O1^{v}	0.894 (19)	2.049 (19)	2.8996 (17)	159 (2)
N8—H8*A*···O3	0.830 (17)	2.367 (18)	3.158 (2)	159 (2)
N8—H8*B*···O7^{iv}	0.867 (19)	2.517 (18)	3.1890 (19)	135 (2)

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH5493).

References

Bruker (2004). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Cook, H. A., Klampfl, C. W. & Buchberger, W. (2005). *Electrophoresis*, **26**, 1576–1583.
Cousson, A., Nicolaï, B. & Fillaux, F. (2005). *Acta Cryst.* E**61**, o222–o224.
Rima, J., Abourida, M., Xu, T., Cho, I. K. & Kyriacos, S. (2008). *J. Food Compost. Anal.* **22**, 689–693.
Sheldrick, G. M. (1996). *SADABS*, University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

supplementary materials

Acta Cryst. (2012). E**68**, o2286 [doi:10.1107/S1600536812029066]

4-Nitrophenol–2,4,6-triamino-1,3,5-triazine–water (2/1/1)

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Comment

Melamines are used in the production of melamine foam in polymeric cleaning (Rima *et al.*, 2008) and as a chemical intermediate in plastics manufacturing (Cook *et al.*, 2005). Here, we report the crystal structure of a the title compound. The asymmetric unit contains one melamine molecule, two independent nitrophenol molecules and one solvent water molecule.

The geometric parameters of the melamine molecule (I) (Fig. 1) are comparable with those determined by Cousson *et al.* (2005). The melamine and nitrophenol molecules are essentially planar, with a maximum deviation of -0.0294 (10) Å for atom N4 in the least square plane (N6/C13/C14/N7/N4/C15/N8/N5), -0.0706 (12) Å for atom O2 in the least square plane (O1/C1-C6/N1/O2/O3) and 0.0742 (12) Å for atom O5 in the least square plane (O4/C10/C11/C12/C7/C8/C9/N2/O5/O6).

In the crystal, O—H···N, N—H···O and O—H···O hydrogen bonds (Table 1 & Fig. 2) and π–π interactions [Cg1···Cg1 (1-x,-y,1-z) distance of 3.749 (3)Å; Cg1···Cg2 (x,-1+y,z) distance of 3.728 (3)Å and Cg2···Cg1 (x,1+y,z) distance of 3.728 (3)Å; Cg1 and Cg2 are the centroids of the rings (C1-C6) and (C7-C12), respectively] connect the components of the structure into a three-dimensional network.

Experimental

Melamine (1.2612g, 0.01 mmol) was dissolved in 200 ml of hot solution of distilled water. p-Nitrophenol (1.3911g, 0.01 mmol) was dissolved in 100 ml of distilled water separately. To the hot solution of melamine, p-nitrophenol solution was added gently, and stirred well for nearly five hours to get the homogenous solution and the mixture is allowed to evaporate. Within a few days tiny, transparent, yellowish crystals were formed. Recrystallization was carried out by using distilled water to get the pure crystal suitable for X-ray diffraction.

Refinement

The H atoms for aromatic C-H groups were positioned geometrically with C–H = 0.93 %A and allowed to ride on their parent atoms, with $U_{iso}(H) = 1.2U_{eq}(C)$ and all other H atoms were located in a difference Fourier map and allowed to refine freely [N—H = 0.830 (17)-0.894 (19)Å and O—H = 0.84 (2)–0.91 (2)Å].

Computing details

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT* (Bruker, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008).

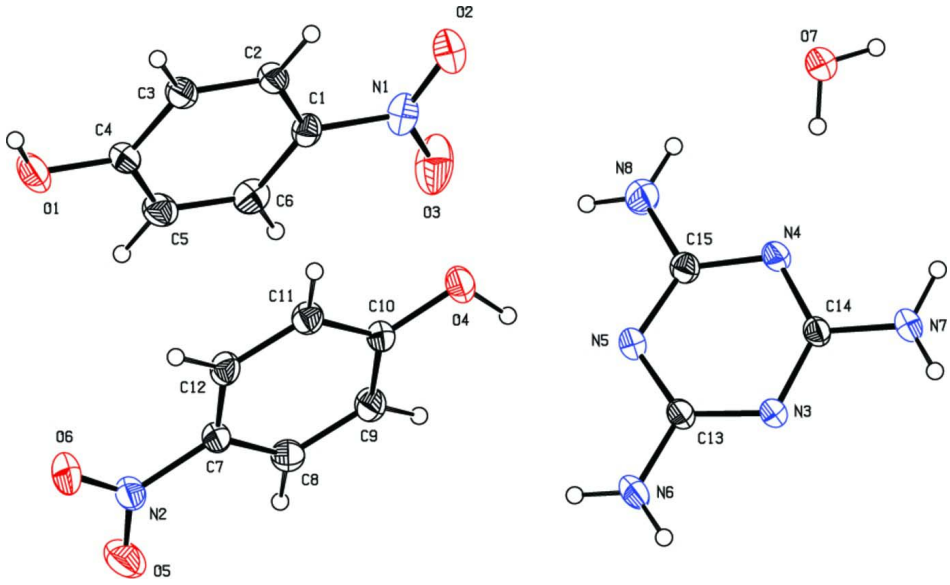

Figure 1

The molecular structure of (I), with 30% probability displacement ellipsoids for non-H atoms.

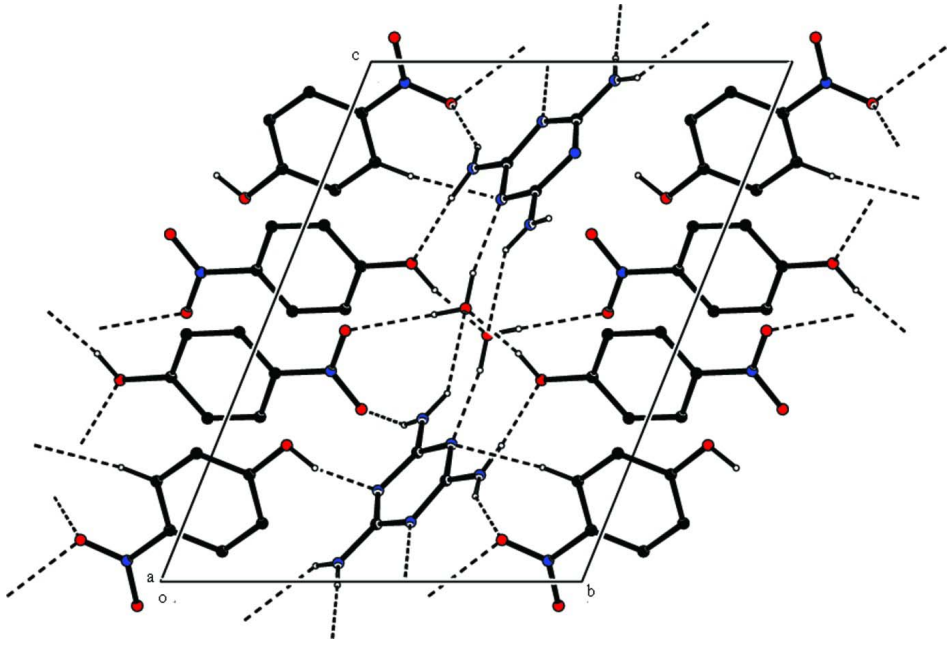

Figure 2

The packing of (I), viewed along the *a* axis. Intermolecular Hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted.

4-Nitrophenol–2,4,6-triamino-1,3,5-triazine–water (2/1/1)

Crystal data

$2C_6H_5NO_3·C_3H_6N_6·H_2O$
$M_r = 422.37$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 7.123$ (5) Å
$b = 10.577$ (4) Å

c = 13.680 (5) Å
α = 68.256 (5)°
β = 88.772 (6)°
γ = 76.604 (5)°
V = 928.9 (8) Å^3
Z = 2
F(000) = 440
D_x = 1.510 Mg m^{-3}

Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 21610 reflections
θ = 2.1–30.7°
μ = 0.12 mm^{-1}
T = 295 K
Block, yellow
0.30 × 0.20 × 0.20 mm

Data collection

Bruker Kappa APEXII diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.964, T_{max} = 0.976

21610 measured reflections
5696 independent reflections
4164 reflections with $I > 2\sigma(I)$
R_{int} = 0.030
θ_{max} = 30.7°, θ_{min} = 2.1°
h = −8→10
k = −15→15
l = −17→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.122
S = 1.03
5696 reflections
311 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0598P)^2 + 0.1276P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
C1	−0.33225 (16)	0.07164 (12)	0.40065 (10)	0.0341 (2)
C2	−0.24544 (16)	−0.05332 (12)	0.48003 (9)	0.0348 (2)
H2	−0.1702	−0.0549	0.5354	0.042*
C3	−0.27246 (18)	−0.17603 (13)	0.47577 (9)	0.0370 (3)
H3	−0.2136	−0.2617	0.5281	0.044*
C4	−0.38715 (18)	−0.17217 (13)	0.39367 (10)	0.0378 (3)
C5	−0.47281 (18)	−0.04548 (15)	0.31426 (10)	0.0423 (3)
H5	−0.5486	−0.0437	0.2590	0.051*
C6	−0.44573 (17)	0.07743 (14)	0.31718 (10)	0.0406 (3)
H6	−0.5024	0.1630	0.2642	0.049*
C7	−0.16167 (17)	−0.02771 (12)	0.09893 (9)	0.0345 (2)
C8	−0.20456 (18)	0.11701 (13)	0.05818 (10)	0.0394 (3)

H8	−0.2801	0.1679	−0.0049	0.047*
C9	−0.13380 (19)	0.18491 (12)	0.11231 (10)	0.0387 (3)
H9	−0.1618	0.2824	0.0860	0.046*
C10	−0.02072 (16)	0.10786 (12)	0.20608 (9)	0.0331 (2)
C11	0.01838 (17)	−0.03791 (12)	0.24690 (10)	0.0357 (2)
H11	0.0921	−0.0892	0.3105	0.043*
C12	−0.05206 (17)	−0.10608 (12)	0.19311 (10)	0.0361 (3)
H12	−0.0263	−0.2035	0.2197	0.043*
C13	0.26472 (17)	0.45692 (12)	0.11080 (9)	0.0339 (2)
C14	0.36186 (16)	0.58004 (11)	0.19500 (9)	0.0305 (2)
C15	0.10688 (16)	0.48525 (11)	0.24878 (9)	0.0322 (2)
N1	−0.30636 (15)	0.20134 (11)	0.40532 (10)	0.0443 (3)
N2	−0.22950 (16)	−0.10017 (13)	0.04030 (9)	0.0447 (3)
N3	0.38541 (14)	0.53546 (10)	0.11487 (7)	0.0338 (2)
N4	0.22586 (14)	0.55802 (10)	0.26462 (7)	0.0329 (2)
N5	0.12224 (14)	0.42855 (10)	0.17511 (8)	0.0359 (2)
N6	0.2906 (2)	0.40378 (15)	0.03568 (10)	0.0538 (3)
N7	0.48129 (18)	0.65529 (12)	0.20504 (10)	0.0444 (3)
N8	−0.03642 (18)	0.46571 (13)	0.31286 (10)	0.0465 (3)
O1	−0.42179 (18)	−0.28988 (12)	0.38794 (9)	0.0562 (3)
O2	−0.21683 (16)	0.19698 (11)	0.48256 (9)	0.0566 (3)
O3	−0.37293 (19)	0.31089 (11)	0.33173 (12)	0.0782 (4)
O4	0.05318 (15)	0.16839 (10)	0.26239 (8)	0.0464 (2)
O5	−0.31476 (16)	−0.03215 (14)	−0.04647 (9)	0.0633 (3)
O6	−0.19394 (18)	−0.22987 (12)	0.08023 (9)	0.0632 (3)
O7	0.23235 (17)	0.53850 (11)	0.47450 (9)	0.0526 (3)
H1	−0.357 (3)	−0.370 (3)	0.4389 (18)	0.093 (7)*
H4	0.054 (3)	0.257 (2)	0.2186 (15)	0.071 (5)*
H6A	0.216 (3)	0.353 (2)	0.0306 (14)	0.063 (5)*
H6B	0.378 (3)	0.4227 (19)	−0.0065 (14)	0.060 (5)*
H7A	0.243 (3)	0.555 (2)	0.4067 (17)	0.075 (6)*
H7B	0.252 (3)	0.607 (2)	0.4863 (17)	0.084 (6)*
H7C	0.576 (2)	0.6648 (17)	0.1643 (13)	0.054 (5)*
H7D	0.478 (2)	0.6781 (18)	0.2619 (15)	0.061 (5)*
H8A	−0.119 (2)	0.4277 (18)	0.3014 (14)	0.058 (5)*
H8B	−0.048 (2)	0.4994 (19)	0.3622 (15)	0.062 (5)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0295 (5)	0.0342 (6)	0.0400 (6)	−0.0099 (4)	0.0057 (4)	−0.0143 (5)
C2	0.0353 (5)	0.0380 (6)	0.0333 (6)	−0.0102 (5)	0.0008 (4)	−0.0151 (5)
C3	0.0442 (6)	0.0343 (6)	0.0329 (6)	−0.0094 (5)	0.0004 (5)	−0.0129 (5)
C4	0.0430 (6)	0.0430 (7)	0.0358 (6)	−0.0153 (5)	0.0064 (5)	−0.0214 (5)
C5	0.0385 (6)	0.0548 (8)	0.0365 (6)	−0.0139 (6)	−0.0014 (5)	−0.0188 (6)
C6	0.0329 (6)	0.0422 (7)	0.0389 (6)	−0.0057 (5)	−0.0015 (5)	−0.0083 (5)
C7	0.0374 (6)	0.0389 (6)	0.0356 (6)	−0.0163 (5)	0.0085 (5)	−0.0195 (5)
C8	0.0446 (6)	0.0391 (6)	0.0321 (6)	−0.0115 (5)	−0.0014 (5)	−0.0098 (5)
C9	0.0485 (7)	0.0279 (5)	0.0376 (6)	−0.0099 (5)	0.0000 (5)	−0.0093 (5)
C10	0.0371 (6)	0.0324 (5)	0.0344 (6)	−0.0131 (4)	0.0055 (4)	−0.0151 (5)

C11	0.0384 (6)	0.0312 (6)	0.0350 (6)	−0.0080 (5)	−0.0002 (5)	−0.0096 (5)
C12	0.0418 (6)	0.0271 (5)	0.0409 (6)	−0.0099 (4)	0.0070 (5)	−0.0135 (5)
C13	0.0448 (6)	0.0315 (5)	0.0297 (5)	−0.0136 (5)	−0.0005 (5)	−0.0134 (5)
C14	0.0394 (6)	0.0249 (5)	0.0281 (5)	−0.0092 (4)	−0.0024 (4)	−0.0100 (4)
C15	0.0380 (6)	0.0265 (5)	0.0317 (5)	−0.0073 (4)	0.0008 (4)	−0.0105 (4)
N1	0.0362 (5)	0.0353 (5)	0.0616 (7)	−0.0111 (4)	0.0050 (5)	−0.0169 (5)
N2	0.0466 (6)	0.0588 (7)	0.0475 (6)	−0.0282 (5)	0.0158 (5)	−0.0326 (6)
N3	0.0446 (5)	0.0344 (5)	0.0288 (5)	−0.0170 (4)	0.0032 (4)	−0.0148 (4)
N4	0.0412 (5)	0.0300 (5)	0.0322 (5)	−0.0104 (4)	0.0028 (4)	−0.0160 (4)
N5	0.0440 (5)	0.0357 (5)	0.0360 (5)	−0.0178 (4)	0.0036 (4)	−0.0175 (4)
N6	0.0714 (8)	0.0706 (8)	0.0509 (7)	−0.0428 (7)	0.0212 (6)	−0.0438 (7)
N7	0.0581 (7)	0.0516 (7)	0.0411 (6)	−0.0309 (6)	0.0084 (5)	−0.0269 (5)
N8	0.0490 (6)	0.0521 (7)	0.0498 (7)	−0.0222 (5)	0.0158 (5)	−0.0265 (6)
O1	0.0798 (7)	0.0498 (6)	0.0523 (6)	−0.0234 (6)	−0.0038 (6)	−0.0293 (5)
O2	0.0633 (6)	0.0503 (6)	0.0687 (7)	−0.0224 (5)	0.0021 (5)	−0.0310 (5)
O3	0.0767 (8)	0.0327 (5)	0.1046 (10)	−0.0105 (5)	−0.0261 (7)	−0.0024 (6)
O4	0.0633 (6)	0.0399 (5)	0.0426 (5)	−0.0224 (4)	−0.0035 (4)	−0.0166 (4)
O5	0.0642 (7)	0.0895 (9)	0.0527 (6)	−0.0272 (6)	−0.0010 (5)	−0.0398 (6)
O6	0.0876 (8)	0.0572 (6)	0.0702 (7)	−0.0425 (6)	0.0180 (6)	−0.0382 (6)
O7	0.0817 (7)	0.0497 (6)	0.0421 (6)	−0.0346 (5)	0.0143 (5)	−0.0242 (5)

Geometric parameters (Å, º)

C1—C2	1.3766 (17)	C13—N6	1.3333 (16)
C1—C6	1.3877 (18)	C13—N3	1.3414 (14)
C1—N1	1.4501 (16)	C13—N5	1.3421 (16)
C2—C3	1.3774 (17)	C14—N7	1.3326 (15)
C2—H2	0.9300	C14—N3	1.3381 (14)
C3—C4	1.3857 (17)	C14—N4	1.3418 (16)
C3—H3	0.9300	C15—N8	1.3335 (17)
C4—O1	1.3538 (15)	C15—N4	1.3384 (15)
C4—C5	1.3852 (19)	C15—N5	1.3416 (15)
C5—C6	1.3726 (19)	N1—O3	1.2176 (16)
C5—H5	0.9300	N1—O2	1.2266 (16)
C6—H6	0.9300	N2—O5	1.2212 (17)
C7—C8	1.3804 (18)	N2—O6	1.2386 (17)
C7—C12	1.3815 (18)	N6—H6A	0.860 (18)
C7—N2	1.4518 (15)	N6—H6B	0.845 (18)
C8—C9	1.3770 (17)	N7—H7C	0.867 (17)
C8—H8	0.9300	N7—H7D	0.894 (19)
C9—C10	1.3871 (18)	N8—H8A	0.830 (17)
C9—H9	0.9300	N8—H8B	0.867 (19)
C10—O4	1.3488 (14)	O1—H1	0.90 (2)
C10—C11	1.3915 (17)	O4—H4	0.91 (2)
C11—C12	1.3747 (17)	O7—H7A	0.88 (2)
C11—H11	0.9300	O7—H7B	0.84 (2)
C12—H12	0.9300		
C2—C1—C6	122.08 (11)	C11—C12—C7	119.00 (11)
C2—C1—N1	118.88 (11)	C11—C12—H12	120.5

C6—C1—N1	119.04 (11)	C7—C12—H12	120.5
C1—C2—C3	118.59 (11)	N6—C13—N3	116.17 (11)
C1—C2—H2	120.7	N6—C13—N5	118.22 (11)
C3—C2—H2	120.7	N3—C13—N5	125.61 (10)
C2—C3—C4	120.13 (11)	N7—C14—N3	117.08 (11)
C2—C3—H3	119.9	N7—C14—N4	117.29 (10)
C4—C3—H3	119.9	N3—C14—N4	125.61 (10)
O1—C4—C5	117.44 (12)	N8—C15—N4	117.07 (11)
O1—C4—C3	122.07 (12)	N8—C15—N5	117.58 (11)
C5—C4—C3	120.48 (11)	N4—C15—N5	125.34 (10)
C6—C5—C4	119.93 (12)	O3—N1—O2	122.26 (12)
C6—C5—H5	120.0	O3—N1—C1	118.70 (12)
C4—C5—H5	120.0	O2—N1—C1	119.04 (11)
C5—C6—C1	118.78 (12)	O5—N2—O6	122.77 (11)
C5—C6—H6	120.6	O5—N2—C7	119.29 (12)
C1—C6—H6	120.6	O6—N2—C7	117.92 (12)
C8—C7—C12	121.83 (10)	C14—N3—C13	114.25 (10)
C8—C7—N2	119.31 (12)	C15—N4—C14	114.57 (10)
C12—C7—N2	118.84 (11)	C15—N5—C13	114.40 (9)
C9—C8—C7	118.99 (11)	C13—N6—H6A	118.8 (12)
C9—C8—H8	120.5	C13—N6—H6B	119.2 (12)
C7—C8—H8	120.5	H6A—N6—H6B	122.0 (17)
C8—C9—C10	119.96 (11)	C14—N7—H7C	118.7 (11)
C8—C9—H9	120.0	C14—N7—H7D	118.9 (11)
C10—C9—H9	120.0	H7C—N7—H7D	121.0 (15)
O4—C10—C9	122.67 (11)	C15—N8—H8A	119.2 (12)
O4—C10—C11	117.05 (11)	C15—N8—H8B	119.5 (11)
C9—C10—C11	120.27 (10)	H8A—N8—H8B	121.1 (16)
C12—C11—C10	119.93 (12)	C4—O1—H1	114.2 (14)
C12—C11—H11	120.0	C10—O4—H4	107.8 (12)
C10—C11—H11	120.0	H7A—O7—H7B	108.7 (19)

C6—C1—C2—C3	0.14 (18)	C2—C1—N1—O3	175.39 (13)
N1—C1—C2—C3	179.25 (11)	C6—C1—N1—O3	−5.47 (18)
C1—C2—C3—C4	−0.89 (18)	C2—C1—N1—O2	−3.93 (17)
C2—C3—C4—O1	−178.18 (11)	C6—C1—N1—O2	175.21 (11)
C2—C3—C4—C5	1.15 (18)	C8—C7—N2—O5	3.71 (17)
O1—C4—C5—C6	178.73 (12)	C12—C7—N2—O5	−174.89 (11)
C3—C4—C5—C6	−0.63 (19)	C8—C7—N2—O6	−177.86 (11)
C4—C5—C6—C1	−0.12 (18)	C12—C7—N2—O6	3.55 (17)
C2—C1—C6—C5	0.37 (18)	N7—C14—N3—C13	178.15 (11)
N1—C1—C6—C5	−178.74 (11)	N4—C14—N3—C13	−3.37 (16)
C12—C7—C8—C9	0.89 (18)	N6—C13—N3—C14	−176.36 (11)
N2—C7—C8—C9	−177.66 (11)	N5—C13—N3—C14	3.84 (17)
C7—C8—C9—C10	0.24 (19)	N8—C15—N4—C14	−177.10 (11)
C8—C9—C10—O4	179.76 (12)	N5—C15—N4—C14	4.13 (17)
C8—C9—C10—C11	−1.32 (18)	N7—C14—N4—C15	178.19 (11)
O4—C10—C11—C12	−179.73 (11)	N3—C14—N4—C15	−0.29 (16)
C9—C10—C11—C12	1.29 (18)	N8—C15—N5—C13	177.51 (11)

C10—C11—C12—C7	−0.18 (18)	N4—C15—N5—C13	−3.73 (17)
C8—C7—C12—C11	−0.92 (18)	N6—C13—N5—C15	179.61 (12)
N2—C7—C12—C11	177.64 (10)	N3—C13—N5—C15	−0.59 (17)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O7^{i}	0.90 (2)	1.76 (2)	2.6600 (18)	172 (2)
O4—H4···N5	0.91 (2)	1.87 (2)	2.7217 (16)	157 (2)
N6—H6*A*···O6^{ii}	0.860 (18)	2.363 (19)	3.0276 (16)	134 (2)
N6—H6*B*···N3^{iii}	0.845 (18)	2.235 (19)	3.080 (2)	178 (2)
O7—H7*A*···N4	0.88 (2)	1.94 (2)	2.8020 (18)	166 (2)
O7—H7*B*···O2^{iv}	0.84 (2)	2.22 (2)	3.0424 (18)	164 (2)
N7—H7*C*···O6^{v}	0.867 (17)	2.250 (17)	3.056 (2)	155 (2)
N7—H7*D*···O1^{v}	0.894 (19)	2.049 (19)	2.8996 (17)	159 (2)
N8—H8*A*···O3	0.830 (17)	2.367 (18)	3.158 (2)	159 (2)
N8—H8*B*···O7^{iv}	0.867 (19)	2.517 (18)	3.1890 (19)	135 (2)

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