

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

1,4-Bis(4,5-dihydro-1H-imidazol-2-yl)-benzene-terephthalic acid-water (1/1/4)

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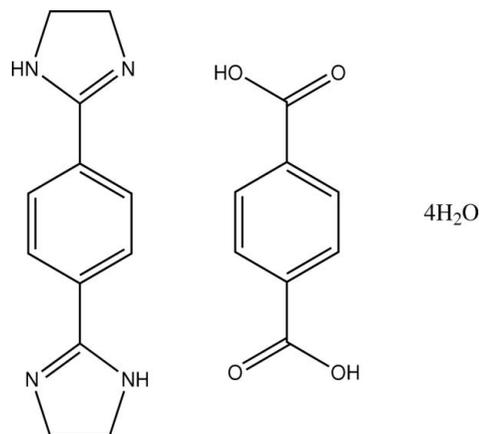
Received 21 September 2009; accepted 6 October 2009

Key indicators: single-crystal X-ray study; $T = 273$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.090; wR factor = 0.257; data-to-parameter ratio = 14.6.

The asymmetric unit of the title compound, $\text{C}_{12}\text{H}_{14}\text{N}_4 \cdot \text{C}_8\text{H}_6\text{O}_4 \cdot 4\text{H}_2\text{O}$, consists of one half of the 1,4-bis(4,5-dihydro-1H-imidazol-2-yl)benzene (bib) molecule, one half of the terephthalic acid (TA) molecule and two water molecules. Both the bib and the TA molecules reside on crystallographic inversion centers, which coincide with the centroids of the respective benzene rings. The bib and the TA, together with the water molecules, are linked through intermolecular $\text{O}-\text{H} \cdots \text{O}$, $\text{O}-\text{H} \cdots \text{N}$ and $\text{N}-\text{H} \cdots \text{O}$ hydrogen bonds, forming a three-dimensional network of stacked layers. Weak intermolecular $\text{C}-\text{H} \cdots \text{O}$ contacts support the stability of the crystal structure.

Related literature

For general background, see: Jeffrey (1997). For hydrogen bonding in molecular complexes of disubstituted biphenyls, see: Thaimattam *et al.* (1998). For the synthesis of the title compound, see: Ren *et al.* (2007). For related structures, see: Ren *et al.* (2007, 2009 and literature cited therein); Shang *et al.* (2009). For experimental refinement details, see: Nardelli, (1999).



Experimental

Crystal data

$\text{C}_{12}\text{H}_{14}\text{N}_4 \cdot \text{C}_8\text{H}_6\text{O}_4 \cdot 4\text{H}_2\text{O}$
 $M_r = 452.46$
 Monoclinic, $P2_1/c$
 $a = 7.9929$ (13) Å
 $b = 16.847$ (3) Å
 $c = 7.9615$ (12) Å
 $\beta = 94.899$ (3)°

$V = 1068.2$ (3) Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 0.11$ mm⁻¹
 $T = 273$ K
 $0.50 \times 0.35 \times 0.30$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
 Absorption correction: multi-scan (SADABS; Bruker, 1998)
 $T_{\min} = 0.947$, $T_{\max} = 0.968$

5588 measured reflections
 2300 independent reflections
 832 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.075$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.090$
 $wR(F^2) = 0.257$
 $S = 0.79$
 2300 reflections
 158 parameters
 6 restraints

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.71$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.43$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H} \cdots A$	$D-\text{H}$	$\text{H} \cdots A$	$D \cdots A$	$D-\text{H} \cdots A$
$\text{O}2\text{W}-\text{H}2\text{WB} \cdots \text{O}1^{\text{i}}$	0.85 (4)	2.37 (6)	2.904 (5)	121 (7)
$\text{O}2\text{W}-\text{H}2\text{WA} \cdots \text{O}1^{\text{ii}}$	0.85	1.96	2.815 (5)	180
$\text{O}1\text{W}-\text{H}1\text{WB} \cdots \text{O}2\text{W}^{\text{iii}}$	0.85 (4)	2.08 (4)	2.926 (5)	172 (5)
$\text{O}1\text{W}-\text{H}1\text{WA} \cdots \text{O}2^{\text{iv}}$	0.86 (3)	1.851 (15)	2.707 (5)	172 (3)
$\text{O}2-\text{H}2\text{D} \cdots \text{N}1$	0.82	2.13	2.934 (4)	165
$\text{N}2-\text{H}2\text{C} \cdots \text{O}1\text{W}^{\text{v}}$	0.86	1.98	2.828 (4)	167
$\text{C}5-\text{H}5 \cdots \text{O}1$	0.93	2.50	3.407 (4)	165
$\text{C}6-\text{H}6 \cdots \text{O}1\text{W}^{\text{v}}$	0.93	2.47	3.380 (6)	166

Symmetry codes: (i) $x, y, z + 1$; (ii) $x, -y + \frac{3}{2}, z + \frac{1}{2}$; (iii) $x, -y + \frac{3}{2}, z - \frac{1}{2}$; (iv) $x + 1, y, z$; (v) $-x + 1, y + \frac{1}{2}, -z + \frac{1}{2}$.

Data collection: SMART (Bruker, 1998); cell refinement: SAINT-Plus (Bruker, 1998); data reduction: SAINT-Plus; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL (Sheldrick, 2008) and PLATON (Spek, 2009); software used to prepare material for publication: SHELXL97

This work was generously supported by the National Natural Science Foundation of China (No. 20701016).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SI2204).

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supporting information

Acta Cryst. (2009). E65, o2682–o2683 [https://doi.org/10.1107/S1600536809040616]

1,4-Bis(4,5-dihydro-1*H*-imidazol-2-yl)benzene–terephthalic acid–water (1/1/4)**Shao-Ming Shang, Su-Yun Li, Chun-Xia Ren, Xin Wang and Lu-De Lu****S1. Comment**

Attention has recently focused on the use of supramolecular interactions such as hydrogen bonding and π – π interactions, in addition to coordinate bonds, in the controlled assembly of supramolecular architectures (Jeffrey, 1997). Hydrogen bonds often play a dominant role in crystal engineering because of their combine strength with directionality (Thaimattam, et al., 1998). On the other hand, supramolecular systems sustained by soft connections, such as hydrogen bonds, are comparatively more flexible and sensitive to the chemical environment. We described previously a number of such complexes, including the imidazole ligand, and have concluded that hydrogen bonding involving this group influences the geometry around the metal atom and the crystallization mechanism [Ren, et al. (2007, 2009 and literature cited therein); Shang et al. (2009)]. We describe herewith the synthesis and crystal structure of the title compound, (Fig. 1), namely bib.TA.4H₂O (I) (bib = 1,4-bis(4,5-dihydro-1*H*-imidazol-2-yl)benzene, TA = terephthalate), which exhibits a three-dimensional hydrogen-bonded molecular architecture.

The crystal lattice contains two bib, two TA and eight lattice water molecules in the solid. The bib and TA in a trans, trans configuration are in a face-to-face orientation and the dihedral angle between acid TA and base bib components is 9.5°. And the bib and TA ligands are joined together by two water molecules through hydrogen bonds between the carboxy oxygen atom in TA and the nitrogen atom of –C=N– in bib to give a macrocycle O1W–H1WB···O2W, O2W–H2WB···O1, O1W–H1WA···O2, N2–H2C···O1W and O2–H2D···N1 with the hydrogen bond geometry given in Table 1, and a face-to-face intracyclic π – π interaction at 3.69 Å (Fig. 1). Each bib group also features another macrocycles, resulting in 1-D chains running along the *a* axis. As illustrated in Fig. 2, the adjacent TA ligands are furthermore linked in the antiparallel alignment with offset along the *ab* plane by hydrogen bonds between the water molecules and the oxygen of TA groups (O2W–H2WA···O1, O1W–H1WA···O2, O2W–H2WB···O1, and O1W–H1WB···O2W (see Table 1). These *ab* planes are packed and stabilized by the hydrogen bonds between the lattice water and oxygen atom of TA ligands (O2w–H2wa···O1 = 2.82 Å) into a 3-D structure. Weak intermolecular C–H···O contacts contribute to the stability of the layered structure (Table 1).

S2. Experimental

All the reagents and solvents employed were commercially available and used as received without further purification.

Syntheses of bib 1,4-Benzenedicarboxylic acid (2.31 g, 13.9 mmol), ethylenediamine (3.70 ml, 50 mmol), ethylenediamine dihydrochloride(6.64 g, 50 mmol) and toluene-*p*-sulfonic acid (0.208 g, 1.09 mmol) were added to the solvent of ethyleneglycol (20 ml), and the mixture solution was refluxed for 3 hr. About half of the ethylene glycol solvent was then slowly removed by distillation. The residue was dissolved in a mixture of water (40 ml) and concentrated HCl (11 *M*, 3 ml). The addition of 50% aqueous NaOH gave a yellow precipitate that was purified by recrystallization. The ligand bib was obtained in 83% based on 1,4-benzenedicarboxylic acid (*ca* 2.50 g). Found: C 66.98; H 6.92; N 26.08%. Calc. for C₁₂H₁₄N₄: C 67.27; H 6.59; N 26.15%. Main IR bonds (KBr, cm⁻¹): 3188*m*, 2936*m*, 2866*m*, 1606 *s*, 1532 *s*, 1466 *s*,

1345*m*, 1270 *s*, 1191*w*, 1080*w*, 981*m*, 907*w*, 767*w*, 687*m*.

Syntheses of bib.TA.4H₂O (I) To a solution of bib (0.043 g, 0.2 mmol) in MeOH (15 ml), an aqueous solution (5 ml) of TA (0.034 g, 0.2 mmol) was added. The solution was allowed at room temperature in air for 48 hr by slow evaporation. Large colourless prismatic crystals of bib.TA.4H₂O were obtained, which were collected by filtration, washed with water and dried in vacuum desiccator over silica gel (0.052 g, 56%). Found: C 53.02; H 6.20; N 12.31%. Calc. for C₁₀H₁₄N₂O₄: C 53.09; H 6.24; N 12.38%. Main IR bonds (KBr,cm⁻¹): 3351*m*, 3142*m*, 2985*m*, 1626 *s*, 1601 *s*, 1582 *s*, 1516*w*, 1366 *s*, 1351 *s*, 1281*m*, 1040*w*, 864*w*, 822*m*, 752*w*, 689*m*.

S3. Refinement

All H atoms attached to C atoms and N atom were fixed geometrically and treated as riding with C—H = 0.93 Å (aromatic) or 0.97 Å (methylene) and N—H = 0.86 Å with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C or N})$. The positions of H atoms for water molecules were calculated (Nardelli, 1999) and included in the subsequent refinement as riding with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$.

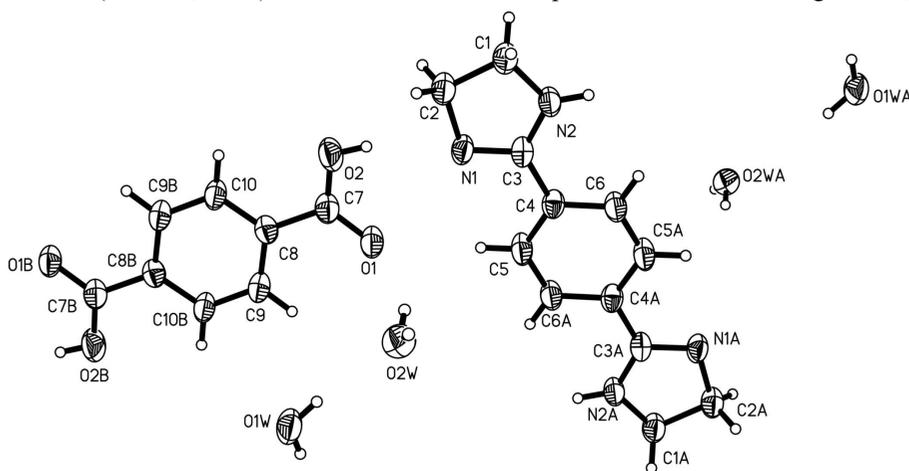


Figure 1

The molecular structure of the title molecule, with the atom-numbering scheme. Symmetry-related atoms shown labelled A and B. [symmetry codes A: $(-x + 1, -y + 2, -z)$; B: $(-x + 1, -y + 1, -z)$].

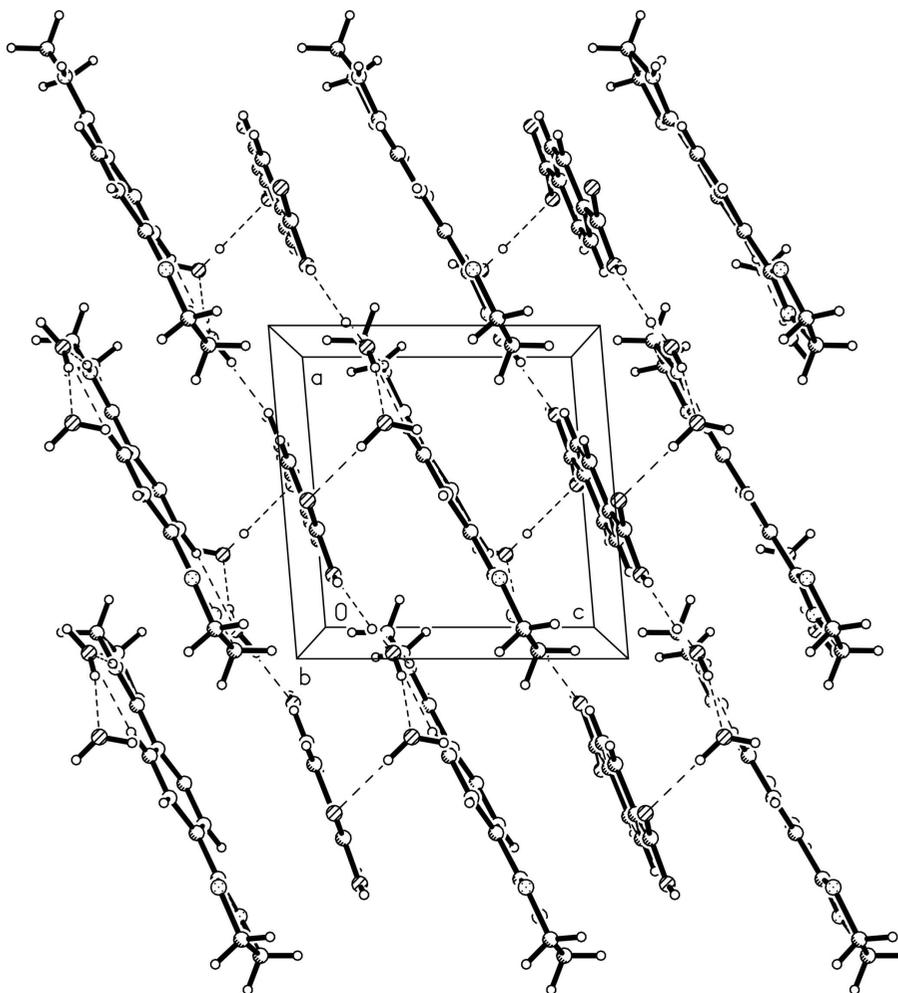


Figure 2

A partial packing diagram for the title compound. Hydrogen bonds are shown as dashed lines.

1,4-Bis(4,5-dihydro-1*H*-imidazol-2-yl)benzene-terephthalic acid-water (1/1/4)

Crystal data

$C_{12}H_{14}N_4 \cdot C_8H_6O_4 \cdot 4H_2O$

$M_r = 452.46$

Monoclinic, $P2_1/c$

$a = 7.9929$ (13) Å

$b = 16.847$ (3) Å

$c = 7.9615$ (12) Å

$\beta = 94.899$ (3)°

$V = 1068.2$ (3) Å³

$Z = 2$

$F(000) = 480$

$D_x = 1.407$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 978 reflections

$\theta = 2.4$ – 22.2 °

$\mu = 0.11$ mm⁻¹

$T = 273$ K

Block, colorless

$0.50 \times 0.35 \times 0.30$ mm

Data collection

Bruker SMART CCD area-detector
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

φ and ω scans

Absorption correction: multi-scan
(*SADABS*; Bruker, 1998)

$T_{\min} = 0.947$, $T_{\max} = 0.968$

5588 measured reflections

2300 independent reflections

832 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.075$
 $\theta_{\text{max}} = 27.0^\circ$, $\theta_{\text{min}} = 2.4^\circ$

$h = -10 \rightarrow 10$
 $k = -21 \rightarrow 21$
 $l = -5 \rightarrow 10$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.090$
 $wR(F^2) = 0.257$
 $S = 0.79$
 2300 reflections
 158 parameters
 6 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
 $w = 1/[\sigma^2(F_o^2) + (0.1628P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.71 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.43 \text{ e } \text{\AA}^{-3}$
 Extinction correction: *SHELXL97* (Sheldrick,
 2008), $F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$
 Extinction coefficient: 0.12 (2)

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness 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 threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
N1	0.2209 (4)	0.83842 (17)	0.1428 (4)	0.0622 (10)
N2	0.0932 (4)	0.95122 (17)	0.1837 (4)	0.0621 (10)
H2C	0.0744	1.0015	0.1797	0.074*
C1	-0.0182 (6)	0.8931 (2)	0.2516 (6)	0.0704 (13)
H1A	-0.1318	0.8981	0.1991	0.085*
H1B	-0.0199	0.8989	0.3726	0.085*
C2	0.0597 (6)	0.8138 (2)	0.2069 (6)	0.0692 (13)
H2A	0.0785	0.7800	0.3053	0.083*
H2B	-0.0109	0.7860	0.1208	0.083*
C3	0.2264 (5)	0.9167 (2)	0.1292 (4)	0.0558 (11)
C4	0.3678 (5)	0.9588 (2)	0.0625 (4)	0.0541 (11)
C5	0.4927 (6)	0.9183 (2)	-0.0102 (5)	0.0684 (13)
H5	0.4886	0.8632	-0.0177	0.082*
O1	0.4731 (4)	0.71811 (16)	0.0453 (4)	0.0702 (9)
O2	0.2324 (5)	0.66542 (18)	0.1033 (4)	0.0915 (11)
H2D	0.2110	0.7124	0.1183	0.137*
C6	0.3758 (6)	1.0410 (2)	0.0723 (5)	0.0659 (12)
H6	0.2921	1.0689	0.1212	0.079*
C7	0.3793 (7)	0.6590 (2)	0.0620 (5)	0.0649 (12)
C8	0.4386 (5)	0.5771 (2)	0.0299 (5)	0.0570 (11)

C9	0.6008 (6)	0.5648 (2)	-0.0226 (5)	0.0647 (12)
H9	0.6694	0.6082	-0.0391	0.078*
C10	0.3416 (6)	0.5107 (2)	0.0509 (5)	0.0644 (12)
H10	0.2339	0.5170	0.0849	0.077*
O1W	0.9737 (5)	0.61448 (19)	0.2736 (5)	0.0901 (12)
H1WA	1.053 (4)	0.627 (2)	0.212 (5)	0.11 (2)*
H1WB	0.904 (5)	0.6509 (19)	0.296 (6)	0.10 (2)*
O2W	0.7204 (4)	0.76340 (18)	0.8161 (5)	0.0821 (11)
H2WA	0.6459	0.7691	0.7341	0.098*
H2WB	0.700 (6)	0.776 (7)	0.916 (3)	0.31 (7)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.076 (2)	0.0398 (17)	0.073 (2)	-0.0058 (16)	0.0184 (18)	0.0054 (15)
N2	0.074 (2)	0.0401 (18)	0.074 (2)	0.0037 (17)	0.0201 (19)	0.0008 (15)
C1	0.082 (3)	0.050 (2)	0.082 (3)	-0.003 (2)	0.021 (2)	0.002 (2)
C2	0.087 (3)	0.047 (2)	0.076 (3)	-0.002 (2)	0.022 (2)	0.0008 (19)
C3	0.078 (3)	0.040 (2)	0.050 (2)	0.000 (2)	0.007 (2)	0.0006 (16)
C4	0.072 (3)	0.043 (2)	0.048 (2)	-0.0032 (19)	0.015 (2)	0.0032 (16)
C5	0.094 (3)	0.039 (2)	0.077 (3)	0.003 (2)	0.033 (3)	-0.003 (2)
O1	0.089 (2)	0.0440 (15)	0.080 (2)	0.0001 (15)	0.0227 (16)	-0.0008 (13)
O2	0.099 (3)	0.0495 (17)	0.132 (3)	0.0123 (16)	0.046 (2)	-0.0028 (16)
C6	0.079 (3)	0.042 (2)	0.081 (3)	0.004 (2)	0.029 (2)	0.0007 (19)
C7	0.080 (3)	0.050 (2)	0.067 (3)	0.003 (2)	0.018 (2)	0.0043 (19)
C8	0.069 (3)	0.047 (2)	0.056 (2)	0.0062 (19)	0.012 (2)	0.0006 (17)
C9	0.082 (3)	0.042 (2)	0.071 (3)	-0.007 (2)	0.011 (2)	-0.0018 (19)
C10	0.080 (3)	0.040 (2)	0.075 (3)	-0.0062 (19)	0.020 (2)	-0.0006 (18)
O1W	0.100 (3)	0.0528 (19)	0.123 (3)	-0.0071 (19)	0.038 (2)	0.0076 (17)
O2W	0.076 (2)	0.077 (2)	0.094 (3)	0.0043 (16)	0.0140 (17)	0.0025 (18)

Geometric parameters (Å, °)

N1—C3	1.324 (5)	O2—C7	1.251 (5)
N1—C2	1.485 (5)	O2—H2D	0.8200
N2—C3	1.319 (5)	C6—C5 ⁱ	1.381 (5)
N2—C1	1.458 (5)	C6—H6	0.9300
N2—H2C	0.8600	C7—C8	1.487 (6)
C1—C2	1.528 (5)	C8—C10	1.379 (5)
C1—H1A	0.9700	C8—C9	1.412 (6)
C1—H1B	0.9700	C9—C10 ⁱⁱ	1.377 (5)
C2—H2A	0.9700	C9—H9	0.9300
C2—H2B	0.9700	C10—C9 ⁱⁱ	1.377 (5)
C3—C4	1.472 (6)	C10—H10	0.9300
C4—C5	1.377 (5)	O1W—H1WA	0.86 (3)
C4—C6	1.389 (5)	O1W—H1WB	0.86 (4)
C5—C6 ⁱ	1.381 (5)	O2W—H2WA	0.85
C5—H5	0.9299	O2W—H2WB	0.85 (4)

O1—C7	1.260 (5)		
C3—N1—C2	110.0 (3)	C4—C5—C6 ⁱ	120.4 (3)
C3—N2—C1	111.2 (3)	C4—C5—H5	119.9
C3—N2—H2C	124.4	C6 ⁱ —C5—H5	119.7
C1—N2—H2C	124.4	C7—O2—H2D	109.5
N2—C1—C2	103.1 (3)	C5 ⁱ —C6—C4	120.5 (4)
N2—C1—H1A	111.1	C5 ⁱ —C6—H6	119.7
C2—C1—H1A	111.1	C4—C6—H6	119.8
N2—C1—H1B	111.1	O2—C7—O1	122.7 (4)
C2—C1—H1B	111.1	O2—C7—C8	116.4 (4)
H1A—C1—H1B	109.1	O1—C7—C8	120.9 (4)
N1—C2—C1	102.7 (3)	C10—C8—C9	117.1 (3)
N1—C2—H2A	111.2	C10—C8—C7	122.8 (4)
C1—C2—H2A	111.2	C9—C8—C7	120.1 (4)
N1—C2—H2B	111.2	C10 ⁱⁱ —C9—C8	120.9 (4)
C1—C2—H2B	111.2	C10 ⁱⁱ —C9—H9	119.6
H2A—C2—H2B	109.1	C8—C9—H9	119.5
N2—C3—N1	112.3 (4)	C9 ⁱⁱ —C10—C8	122.0 (4)
N2—C3—C4	124.9 (3)	C9 ⁱⁱ —C10—H10	118.8
N1—C3—C4	122.8 (4)	C8—C10—H10	119.1
C5—C4—C6	119.1 (4)	H1WA—O1W—H1WB	118 (2)
C5—C4—C3	121.3 (3)	H2WA—O2W—H2WB	120.8
C6—C4—C3	119.6 (4)		
C3—N2—C1—C2	-7.5 (4)	C3—C4—C5—C6 ⁱ	179.9 (4)
C3—N1—C2—C1	-7.6 (4)	C5—C4—C6—C5 ⁱ	-0.1 (7)
N2—C1—C2—N1	8.6 (4)	C3—C4—C6—C5 ⁱ	-179.9 (4)
C1—N2—C3—N1	2.9 (5)	O2—C7—C8—C10	-2.8 (6)
C1—N2—C3—C4	-176.3 (4)	O1—C7—C8—C10	178.3 (4)
C2—N1—C3—N2	3.3 (5)	O2—C7—C8—C9	177.9 (4)
C2—N1—C3—C4	-177.5 (3)	O1—C7—C8—C9	-1.0 (6)
N2—C3—C4—C5	-172.2 (4)	C10—C8—C9—C10 ⁱⁱ	-0.1 (6)
N1—C3—C4—C5	8.6 (6)	C7—C8—C9—C10 ⁱⁱ	179.2 (4)
N2—C3—C4—C6	7.6 (6)	C9—C8—C10—C9 ⁱⁱ	0.1 (6)
N1—C3—C4—C6	-171.6 (4)	C7—C8—C10—C9 ⁱⁱ	-179.2 (4)
C6—C4—C5—C6 ⁱ	0.1 (7)		

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

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O2W—H2WB...O1 ⁱⁱⁱ	0.85 (4)	2.37 (6)	2.904 (5)	121 (7)
O2W—H2WA...O1 ^{iv}	0.85	1.96	2.815 (5)	180
O1W—H1WB...O2W ^v	0.85 (4)	2.08 (4)	2.926 (5)	172 (5)
O1W—H1WA...O2 ^{vi}	0.86 (3)	1.85 (2)	2.707 (5)	172 (3)
O2—H2D...N1	0.82	2.13	2.934 (4)	165

N2—H2C···O1 \mathcal{W}^{ii}	0.86	1.98	2.828 (4)	167
C5—H5···O1	0.93	2.50	3.407 (4)	165
C6—H6···O1 \mathcal{W}^{vi}	0.93	2.47	3.380 (6)	166

Symmetry codes: (iii) $x, y, z+1$; (iv) $x, -y+3/2, z+1/2$; (v) $x, -y+3/2, z-1/2$; (vi) $x+1, y, z$; (vii) $-x+1, y+1/2, -z+1/2$.