

Crystal structure of a new molecular salt: 4-aminobenzenaminium 5-carboxypentanoate

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Keywords: crystal structure; *p*-phenylenediamine; adipic acid; mechanochemical synthesis; LAG; partial protonation; hydrogen bonding.

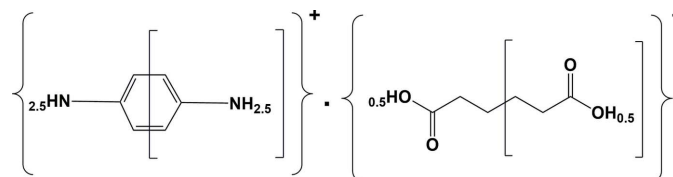
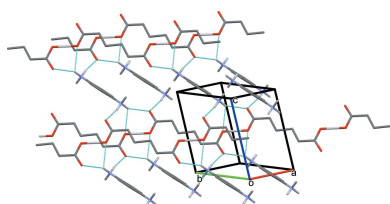
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The asymmetric unit of the title molecular salt (systematic name: 4-aminoanilinium 5-carboxypentanoate), $C_6H_9N_2^+ \cdot C_6H_9O_4^-$, consists of half a 4-aminobenzenaminium cation (4-ABA) and half a 5-carboxypentanoate anion (5-CP); the other half of each ion is generated by inversion symmetry. Protonation of *p*-phenylenediamine (PPDA) leads to the formation of a 1:1 salt, but scrutiny of the crystal structure reveals that both of the amine groups of PPDA are partially protonated, with a half-occupied H atom. For the 5-CP anion, an H atom is positioned on an inversion center midway between two O atoms of inversion-related 5-CP ions. In the crystal, the 5-CP anions are linked by the $O-H \cdots O$ hydrogen bond to form chains propagating along the $[1\bar{1}0]$ direction. The chains are linked *via* $N-H \cdots O$ and $N-H \cdots N$ hydrogen bonds involving the 4-ABA cations, forming a three-dimensional supramolecular framework. The title salt was also prepared by mechanochemical synthesis using liquid-assisted grinding (LAG). Its PXRD pattern matches that of the simulated pattern of the crystal structure of the title molecular salt.

1. Chemical context

p-Phenylenediamine (PPDA) has been widely used to synthesize hair dyes, engineering polymers and composites. The coordination chemistry of PPDA is well documented (Adams *et al.*, 2011; Bourne & Mangombo, 2004). Adipic acid (AA) is an industrial chemical used to manufacture nylon and is also used in many drugs and food additives (Rowe *et al.*, 2009). A number of salts and co-crystals involving *p*-phenylenediamine have been reported (Thakuria *et al.*, 2007; Delori *et al.*, 2016), and adipic acid is also widely known as a co-former in co-crystal formation (Swinton Darious *et al.*, 2016; Lemmerer *et al.*, 2012; Lin *et al.*, 2012; Matulková *et al.*, 2014; Thanigaimani *et al.*, 2012). A 2:1 salt of 4-aminoanilinium (PPDAH) and sebacate, and a 1:1 salt of PPDAH and dihydrogen trimesate have been reported recently (Delori *et al.*, 2016). We have previously reported various salts of *o*-phenylenediamine with aromatic carboxylic acids (Mishra & Pallepogu, 2018). Herein, we report on the synthesis and crystal structure of the 1:1 salt formed between *p*-phenylenediamine and adipic acid, (I).



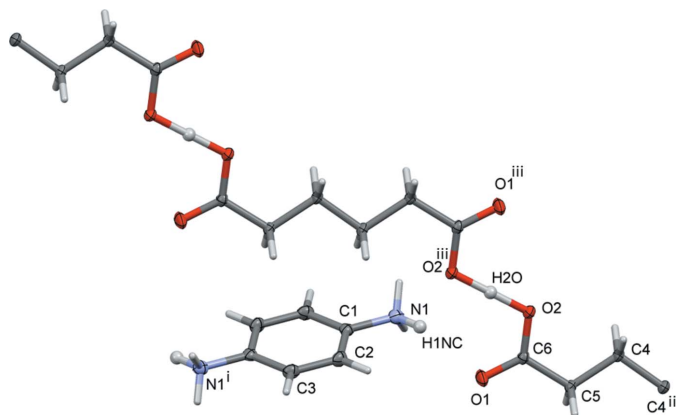


Figure 1
The molecular structure of the title molecular salt (I), with atom labelling for the asymmetric unit. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry codes: (i) $-x + 1, -y + 2, -z + 2$; (ii) $-x + 2, -y, -z + 1$; (iii) $-x + 1, -y + 1, -z + 1$].

2. Structural commentary

The asymmetric unit of the title salt (I), illustrated in Fig. 1, consists of half each of a 4-aminobenzenaminium cation (4-ABA) and a 5-carboxypentanoate anion (5-CP); both ions (space group $P\bar{1}$) lie about inversion centres. Partial protonation (50%) has occurred at atom N1 of the cation, resulting in the formation of a salt with the formula unit $C_6H_9O_4^- \cdot C_6H_9N_2^+$. One of the two adipic acid H atoms binds to atom N1 with a site-occupancy factor (SOF) of 0.5 (for atom H1NC), thereby positioned at two sites (because of inversion symmetry) in the cation. The other acid H atom (H2O) is located on an inversion center and is therefore shared equally by two O2 atoms of inversion-related anions. The C1–N1 bond length [1.4361 (13) Å] in the 4-ABA cation is longer than literature values for a non-protonated amine (C–NH₂) group [*cf.* 1.418 (2) Å; Czapik *et al.*, 2010] and this can be attributed to the partial protonation with SOF = 0.50 at each site. In the 5-CP anion, the C6=O1 and C6–O2 bond lengths [1.2379 (12) and 1.2802 (11) Å, respectively] are similar to the values reported for 2-methylimidazolium hydrogen adipate monohydrate [1.244 (2) and 1.264 (2) Å, respectively; Meng *et al.*, 2009] in which a carboxylic acid H atom is also statistically distributed between the two carboxy groups and a hydrogen-bonded chain is formed. In (I), the position of this H atom (H2O) was located in a difference-Fourier map and found to be situated on an inversion centre ($\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$). It is positioned symmetrically between two O2 atoms of two inversion-related 5-CP ions, which accounts for the long O–H bond length of 1.22 Å (see Table 1). The C4ⁱⁱ–C4–C5–C6 torsion angle of -179.82 (9)° indicates that the carbon chain in the anion is fully extended [see Fig. 1 for symmetry code (ii)].

3. Supramolecular features

In general, adipic acid (AA) forms $R_2^2(8)$ homosynthons facilitated by strong O–H···O interactions; however, it is known to form heterosynthons when co-crystallized with

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

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O2–H2O···O2 ⁱ	1.22	1.22	2.439 (1)	180
O2–H2O···O1 ⁱ	1.22	2.45	3.178 (1)	116
N1–H1NA···O1 ⁱⁱ	0.91 (2)	1.97 (2)	2.871 (1)	171 (1)
N1–H1NB···O1	0.90 (2)	2.24 (2)	3.060 (1)	152 (1)
N1–H1NB···O2 ⁱ	0.90 (2)	2.51 (2)	3.098 (1)	123 (1)
N1–H1NC···N1 ⁱⁱⁱ	0.95 (2)	1.89 (2)	2.840 (1)	174 (2)

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

amines (Lemmerer *et al.*, 2010, 2012). In the crystal structure of (I), the formation of the $R_2^2(8)$ homosynthon is not favoured because of the inversion-related arrangement of the 5-CP anions, which forms a linear chain along the $[1\bar{1}0]$ direction (Fig. 2, Table 1) as a result of the sharing of the H atom (H2O) between the O2 atoms of inversion-related anions as discussed above; otherwise this could be supposed to be the contribution of a strong O–H···O hydrogen bond. The crystal structure features interionic N–H···O and O–H···O hydrogen bonds between the anions and cations (Table 1, Fig. 3). One of the H atoms (H1BA) on N1 is a bifurcated hydrogen-bond donor and the carboxylate O1 atom of the anion acts as a triple acceptor, accepting H atoms from two different NH₃ groups (H1NA and H1NB), as illustrated in Fig. 3. The chains of the 5-CP anions are linked *via* the N–H···O, O–H···O and N–H···N hydrogen bonds, forming a three-dimensional supramolecular framework (Table 1 and Fig. 4).

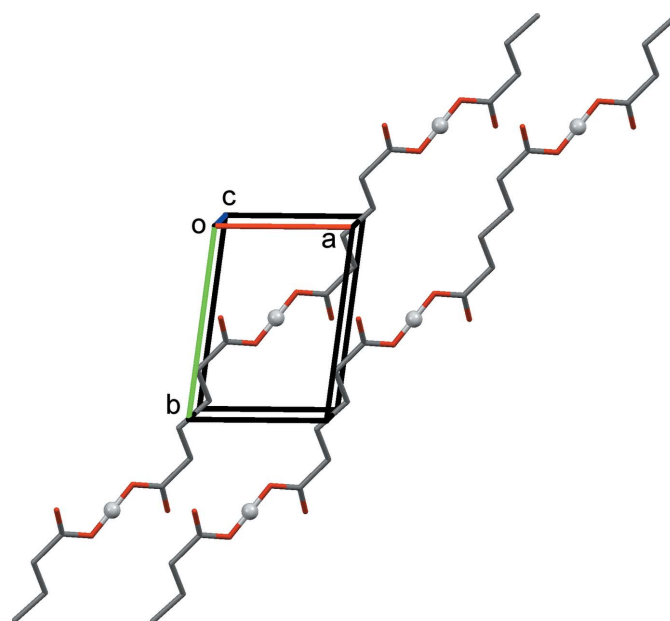


Figure 2
A view along the c axis of the O–H···O hydrogen-bonded chain of 5-CP anions (see Table 1). The H atoms (H2O; shown as grey balls) are shared between O2 atoms of inversion-related anions. The C-bound H atoms and the cations have been omitted.

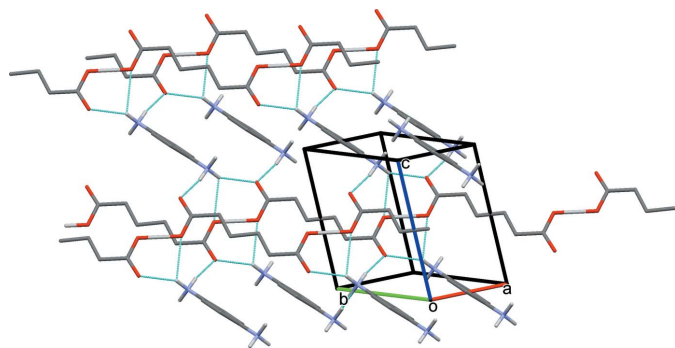


Figure 3
A partial view, normal to the *ab* plane, of the crystal packing of the title molecular salt (I). Hydrogen bonds are shown as dashed lines (see Table 1), and C-bound H atoms have been omitted for clarity.

4. Database survey

A search of the Cambridge Structural Database (CSD, Version 5.38, update May 2017; Groom *et al.*, 2016) for 4-aminoanilinium and 1,4-phenylenediammonium salts gave 70 hits. The crystal structure of *p*-phenylenediamine (PPDA) itself was first reported by Poveteva & Zvonkova (1975). Perhaps the most relevant hit is for the structure of bis(4-aminoanilinium) decanedioate (CSD refcode IPAPAS; Delori *et al.*, 2016), one of the few salts formed with an aliphatic diacid. There are a number of structures reported of PPDA

with mineral acids (Chandrasekaran, 1969; Marsh, 2009; Anderson *et al.*, 2006), and co-crystals and salts of PPDA with organic acids (Thakuria *et al.*, 2007; Delori *et al.*, 2016). Some 1:1 co-crystals of PPDA and various diols (*viz.* 1,8-octane diol, 1,10-decane diol and 1,12-dodecane diol) have also been reported (Loehlin & Okasako, 2007).

A search of the CSD for salts of adipic acid (AA) with different amines yielded 67 hits. One such structure of particular interest, *viz.* 2-methylimidazolium hydrogen adipate monohydrate, has been reported twice, once at room temperature (BOTTOU: Meng *et al.*, 2009), where the same type of partial disorder is observed with the carboxylic acid H atom statistically distributed between the two carboxy groups and a hydrogen-bonded chain is formed. However, the low-temperature analysis at 120 K using synchrotron radiation (BOTTOU01: Callear *et al.*, 2010), describes the structure as bis(2-methylimidazolium) adipate adipic acid dihydrate. In the crystal, the adipate and adipic acid molecules also form a hydrogen-bonded chain. A second structure, tetrakis(cytosinium) dihydrogen bis(adipate), also exhibits the same type of disorder of the carboxylic acid H atom (OYEREQ; Das & Baruah, 2011), and in the crystal it forms a hydrogen-bonded chain.

5. Synthesis and crystallization

The title molecular salt (I), was synthesized by mixing a 5 ml methanolic solution of adipic acid (AA: 0.5 mmol, 73 mg) and 3 ml of an acetonitrile solution of *p*-phenylenediamine (PPDA: 0.5 mmol, 54 mg). The reaction mixture was heated to 323 K with magnetic stirring for *ca* 30 min, and then filtered and allowed to evaporate slowly at room temperature. Purple block-like crystals of (I) were obtained after 5 d (m.p. 438 K). FTIR (KBr pellet, cm^{-1}): ν 3337, 3180, 2946, 2383, 1706, 1515, 1255, 821, 743, 501, 475.

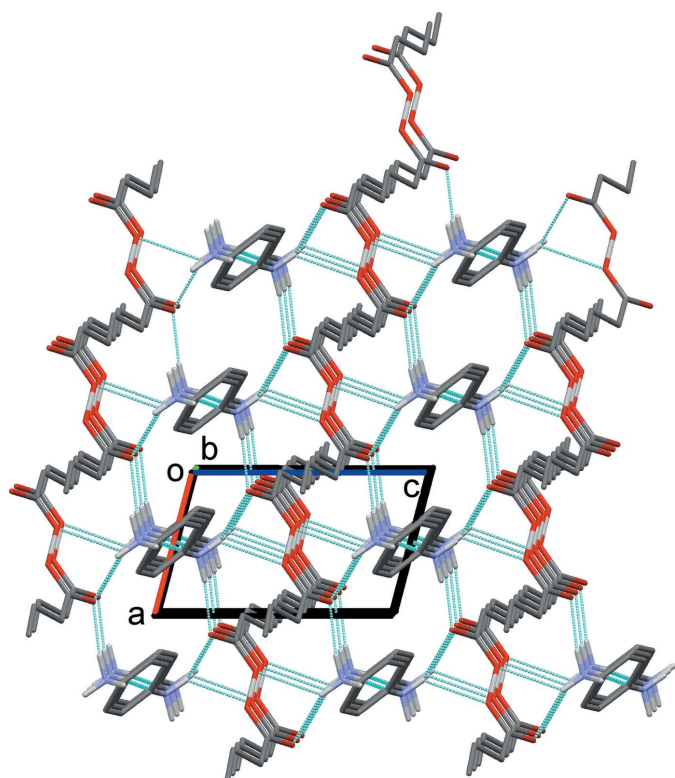


Figure 4
A view along the *b* axis of the crystal packing of the title molecular salt (I), showing the three-dimensional supramolecular framework. Hydrogen bonds are shown as dashed lines (see Table 1), and C-bound H atoms have been omitted for clarity.

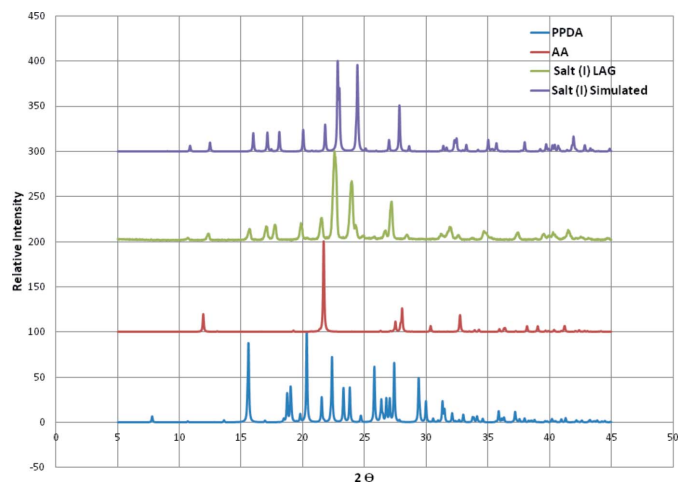


Figure 5
The PXRD pattern obtained from the product of the LAG experiment, and the simulated PXRD pattern of the crystal structure of the title molecular salt. The PXRD patterns of the reactants used for the co-crystallization and LAG syntheses are also shown.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_6H_9N_2^+ \cdot C_6H_9O_4^-$
M_r	254.28
Crystal system, space group	Triclinic, $P\bar{1}$
Temperature (K)	100
a, b, c (Å)	5.2918 (3), 7.1666 (4), 8.4205 (7)
α, β, γ (°)	92.069 (6), 104.165 (6), 97.172 (5)
V (Å ³)	306.47 (4)
Z	1
Radiation type	Mo $K\alpha$
μ (mm ⁻¹)	0.10
Crystal size (mm)	0.42 × 0.38 × 0.32
Data collection	
Diffractometer	Rigaku Oxford Diffraction XtaLAB Pro: Kappa dual offset/ far
Absorption correction	Multi-scan (<i>CrysAlis PRO</i> ; Rigaku OD, 2015)
T_{\min}, T_{\max}	0.924, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	3776, 1416, 1341
R_{int}	0.015
$(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹)	0.685
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.034, 0.092, 1.08
No. of reflections	1416
No. of parameters	96
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å ⁻³)	0.39, -0.22

Computer programs: *CrysAlis PRO* (Rigaku OD, 2015), *SHELXS97* (Sheldrick, 2008), *SHELXL2016/6* (Sheldrick, 2015), *OLEX2* (Dolomanov *et al.*, 2009), *Mercury* (Macrae *et al.*, 2008), *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

The title compound was also synthesized by liquid-assisted grinding (LAG). For this mechanochemical synthesis, equimolar amounts of AA (1 mmol, 146 mg) and PPDA (1 mmol, 108 mg) were ground for 20 min. in a mortar and pestle using 3 to 4 drops of acetonitrile. The powdered sample was collected for PXRD and the resultant pattern was scrutinized for new peaks, as evidence for the formation of the title molecular salt (I), by comparing this pattern with the simulated pattern obtained from the CIF file of salt (I). The PXRD pattern of the compound obtained from the LAG experiment matches the simulated pattern obtained for (I), formed by co-crystallization (Fig. 5).

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. C-bound H atoms were placed in calculated positions and refined using a riding-model approximation: 0.95–0.99 Å with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. The ammonium and carboxyl H atoms were located in difference-Fourier maps and were freely refined. The H atom (H1NC) bound to N1 of the 4-ABA cation, with an occupancy factor of 0.5, is positioned at two sites of the cation due to inversion symmetry, giving rise to a monoprotinated species. The carboxylic acid H atom (H2O) is positioned symmetrically

between the two O2 atoms of inversion-related 5-CP ions (H–O = 1.22 Å). This H atom (H2O) is located on an inversion center ($\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$) with an occupancy factor of 0.5, and hence gives rise to a mono-deprotonated species.

Acknowledgements

The authors thank Professor B. R. Srinivasan, Goa University and Dr N. Jagadeesh Babu, ICT, Hyderabad for useful discussions.

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Acta Cryst. (2018). E74, 201-205 [https://doi.org/10.1107/S2056989018000737]

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Computing details

Data collection: *CrysAlis PRO* (Rigaku OD, 2015); cell refinement: *CrysAlis PRO* (Rigaku OD, 2015); data reduction: *CrysAlis PRO* (Rigaku OD, 2015); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2016/6* (Sheldrick, 2015); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009) and *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXL2016/6* (Sheldrick, 2015), *OLEX2* (Dolomanov *et al.*, 2009), *PLATON* (Spek, 2009) and *publCIF* (Westrip (2010)).

4-Aminoanilinium 5-carboxypentanoate

Crystal data

$\text{C}_6\text{H}_9\text{N}_2^+\cdot\text{C}_6\text{H}_9\text{O}_4^-$
 $M_r = 254.28$
 Triclinic, $P\bar{1}$
 $a = 5.2918$ (3) Å
 $b = 7.1666$ (4) Å
 $c = 8.4205$ (7) Å
 $\alpha = 92.069$ (6)°
 $\beta = 104.165$ (6)°
 $\gamma = 97.172$ (5)°
 $V = 306.47$ (4) Å³

$Z = 1$
 $F(000) = 136$
 $D_x = 1.378$ Mg m⁻³
 Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
 Cell parameters from 5347 reflections
 $\theta = 5.2\text{--}29.2^\circ$
 $\mu = 0.10$ mm⁻¹
 $T = 100$ K
 Block, purple
 $0.42 \times 0.38 \times 0.32$ mm

Data collection

Rigaku Oxford Diffraction XtaLAB Pro: Kappa dual offset/far diffractometer
 Radiation source: fine-focus sealed X-ray tube, Enhance (Mo) X-ray Source
 Graphite monochromator
 ω scans
 Absorption correction: multi-scan (CrysAlis PRO; Rigaku OD, 2015)

$T_{\min} = 0.924$, $T_{\max} = 1.000$
 3776 measured reflections
 1416 independent reflections
 1341 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.015$
 $\theta_{\text{max}} = 29.1^\circ$, $\theta_{\text{min}} = 5.0^\circ$
 $h = -5 \rightarrow 7$
 $k = -9 \rightarrow 8$
 $l = -11 \rightarrow 10$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.034$
 $wR(F^2) = 0.092$
 $S = 1.08$
 1416 reflections

96 parameters
 0 restraints
 Primary atom site location: structure-invariant direct methods
 Secondary atom site location: difference Fourier map

Hydrogen site location: mixed
 H atoms treated by a mixture of independent
 and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.0483P)^2 + 0.0998P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.39 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.22 \text{ e } \text{\AA}^{-3}$
 Extinction correction: (SHELXL-2016/6;
 Sheldrick, 2015),
 $F_c^* = kFc[1 + 0.001x Fc^2 \lambda^3 / \sin(2\theta)]^{-1/4}$
 Extinction coefficient: 0.15 (2)

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
O1	0.88613 (16)	0.51078 (11)	0.73311 (10)	0.0284 (2)	
O2	0.62365 (13)	0.36690 (9)	0.50333 (8)	0.0159 (2)	
H2O	0.500000	0.500000	0.500000	0.079 (10)*	
C4	0.90322 (17)	0.07097 (12)	0.49487 (11)	0.0140 (2)	
H4A	0.867169	0.119848	0.384244	0.017*	
H4B	0.735161	0.007357	0.511087	0.017*	
C5	1.01023 (17)	0.23441 (12)	0.62353 (11)	0.0127 (2)	
H5A	1.048177	0.183438	0.733310	0.015*	
H5B	1.178973	0.295883	0.606644	0.015*	
C6	0.82994 (17)	0.38253 (12)	0.62270 (11)	0.0122 (2)	
N1	0.43897 (17)	0.62290 (12)	0.87167 (10)	0.0177 (2)	
H1NA	0.268 (3)	0.582 (2)	0.8186 (19)	0.033 (4)*	
H1NB	0.538 (3)	0.608 (2)	0.800 (2)	0.036 (4)*	
H1NC	0.470 (5)	0.534 (3)	0.953 (3)	0.013 (6)*	0.5
C1	0.47080 (18)	0.81542 (13)	0.93517 (11)	0.0147 (2)	
C2	0.65701 (19)	0.95024 (15)	0.89941 (12)	0.0180 (2)	
H2	0.764255	0.916272	0.830590	0.022*	
C3	0.68658 (19)	1.13477 (14)	0.96421 (12)	0.0179 (2)	
H3	0.814280	1.227114	0.939883	0.021*	

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0309 (4)	0.0199 (4)	0.0270 (4)	0.0138 (3)	-0.0099 (3)	-0.0120 (3)
O2	0.0149 (4)	0.0149 (3)	0.0169 (4)	0.0069 (3)	0.0000 (3)	-0.0023 (3)
C4	0.0124 (4)	0.0124 (4)	0.0173 (5)	0.0051 (3)	0.0023 (3)	-0.0011 (3)
C5	0.0108 (4)	0.0119 (4)	0.0154 (4)	0.0034 (3)	0.0027 (3)	0.0006 (3)
C6	0.0131 (4)	0.0101 (4)	0.0144 (4)	0.0023 (3)	0.0049 (3)	0.0015 (3)
N1	0.0164 (4)	0.0225 (4)	0.0144 (4)	0.0030 (3)	0.0040 (3)	0.0012 (3)
C1	0.0137 (4)	0.0187 (5)	0.0107 (4)	0.0033 (3)	0.0009 (3)	0.0006 (3)
C2	0.0160 (4)	0.0246 (5)	0.0154 (4)	0.0041 (4)	0.0070 (3)	0.0008 (4)
C3	0.0149 (4)	0.0223 (5)	0.0172 (5)	0.0003 (4)	0.0064 (4)	0.0023 (4)

Geometric parameters (Å, °)

O1—C6	1.2379 (12)	N1—C1	1.4361 (13)
O2—C6	1.2802 (11)	N1—H1NA	0.914 (17)
O2—H2O	1.2197 (6)	N1—H1NB	0.906 (17)
C4—C5	1.5195 (12)	N1—H1NC	0.95 (2)
C4—C4 ⁱ	1.5213 (16)	C1—C2	1.3870 (14)
C4—H4A	0.9900	C1—C3 ⁱⁱ	1.3916 (13)
C4—H4B	0.9900	C2—C3	1.3876 (14)
C5—C6	1.5123 (12)	C2—H2	0.9500
C5—H5A	0.9900	C3—H3	0.9500
C5—H5B	0.9900		
C6—O2—H2O	113.50 (6)	C1—N1—H1NA	111.1 (9)
C5—C4—C4 ⁱ	111.39 (9)	C1—N1—H1NB	111.9 (10)
C5—C4—H4A	109.3	H1NA—N1—H1NB	107.8 (14)
C4 ⁱ —C4—H4A	109.3	C1—N1—H1NC	114.7 (15)
C5—C4—H4B	109.3	H1NA—N1—H1NC	101.0 (18)
C4 ⁱ —C4—H4B	109.3	H1NB—N1—H1NC	109.6 (18)
H4A—C4—H4B	108.0	C2—C1—C3 ⁱⁱ	120.02 (9)
C6—C5—C4	115.04 (8)	C2—C1—N1	121.06 (8)
C6—C5—H5A	108.5	C3 ⁱⁱ —C1—N1	118.91 (9)
C4—C5—H5A	108.5	C1—C2—C3	119.97 (9)
C6—C5—H5B	108.5	C1—C2—H2	120.0
C4—C5—H5B	108.5	C3—C2—H2	120.0
H5A—C5—H5B	107.5	C2—C3—C1 ⁱⁱ	120.01 (9)
O1—C6—O2	123.47 (8)	C2—C3—H3	120.0
O1—C6—C5	120.06 (8)	C1 ⁱⁱ —C3—H3	120.0
O2—C6—C5	116.47 (8)		
C4 ⁱ —C4—C5—C6	−179.82 (9)	C3 ⁱⁱ —C1—C2—C3	0.09 (16)
C4—C5—C6—O1	172.41 (9)	N1—C1—C2—C3	−179.06 (9)
C4—C5—C6—O2	−8.04 (12)	C1—C2—C3—C1 ⁱⁱ	−0.10 (16)

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

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
O2—H2O \cdots O2 ⁱⁱⁱ	1.22	1.22	2.439 (1)	180
O2—H2O \cdots O1 ⁱⁱⁱ	1.22	2.45	3.178 (1)	116
N1—H1NA \cdots O1 ^{iv}	0.91 (2)	1.97 (2)	2.871 (1)	171 (1)
N1—H1NB \cdots O1	0.90 (2)	2.24 (2)	3.060 (1)	152 (1)
N1—H1NB \cdots O2 ⁱⁱⁱ	0.90 (2)	2.51 (2)	3.098 (1)	123 (1)
N1—H1NC \cdots N1 ^v	0.95 (2)	1.89 (2)	2.840 (1)	174 (2)

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