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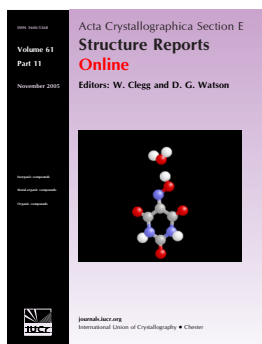
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N'-Acetyl-5-amino-1-methyl-1*H*-pyrazole-4-carbohydrazonamide dihydrate

Anna V. Dolzhenko, Anton V. Dolzhenko, Geok Kheng Tan, Lip Lin Koh
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N'-Acetyl-5-amino-1-methyl-1*H*-pyrazole-4-carbohydrazonamide dihydrate

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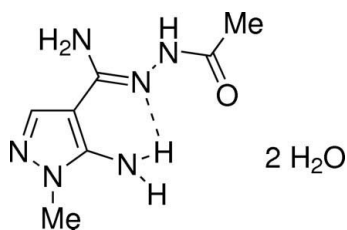
Received 22 April 2010; accepted 26 April 2010

Key indicators: single-crystal X-ray study; $T = 223$ K; mean $\sigma(C-C) = 0.003$ Å; R factor = 0.052; wR factor = 0.141; data-to-parameter ratio = 13.9.

In the title compound, $C_7H_{12}N_6O \cdot 2H_2O$, the *Z* configuration of the hydrazone fragment is stabilized by an intramolecular $N-H \cdots N$ hydrogen bond involving one of the amino groups. In the crystal structure, the hydrazonamide molecules are connected *via* intermolecular $N-H \cdots O=C$ hydrogen bonds, forming *C*(7) chains running along [010]. The chains form sheets parallel to the (101). The chains are cross-linked by water molecules to form a three-dimensional hydrogen-bonded network.

Related literature

For bioactive pyrazoles, see: Elguero *et al.* (2002); Lamberth (2007). For the use of pyrazoles as synthons in heterocyclic chemistry, see: Schenone *et al.* (2007); Dolzhenko *et al.* (2008). For the use of pyrazoles in metal-organic chemistry, see: Mukherjee (2000); Halcrow (2009). For the crystal structures of related 5-amino-1*H*-pyrazole-4-carboxylic acid derivatives, see: Zia-ur-Rehman *et al.* (2008, 2009); Caruso *et al.* (2009). For the crystal structure of *N'*-acetyl-2-phenylethanehydrazonamide, see: Ianelli *et al.* (2001). For the graph-set analysis of hydrogen bonding, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$C_7H_{12}N_6O \cdot 2H_2O$
 $M_r = 232.26$
 Triclinic, $P\bar{1}$
 $a = 7.5496$ (9) Å
 $b = 7.6208$ (9) Å
 $c = 11.2518$ (13) Å
 $\alpha = 102.645$ (2)°
 $\beta = 101.440$ (2)°

$\gamma = 110.810$ (2)°
 $V = 562.75$ (11) Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 0.11$ mm⁻¹
 $T = 223$ K
 $0.45 \times 0.12 \times 0.10$ mm

Data collection

Bruker SMART APEX CCD diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 2001)
 $T_{min} = 0.953$, $T_{max} = 0.989$

3963 measured reflections
 2548 independent reflections
 2174 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.021$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.052$
 $wR(F^2) = 0.141$
 $S = 1.05$
 2548 reflections
 183 parameters

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{max} = 0.31$ e Å⁻³
 $\Delta\rho_{min} = -0.26$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

| $D-H \cdots A$ | $D-H$ | $H \cdots A$ | $D \cdots A$ | $D-H \cdots A$ |
|---------------------------|----------|--------------|--------------|----------------|
| $O2W-H4W \cdots N1^i$ | 0.87 (3) | 2.04 (3) | 2.884 (2) | 162 (3) |
| $O2W-H3W \cdots O1$ | 0.86 (3) | 2.11 (3) | 2.885 (2) | 150 (3) |
| $O1W-H2W \cdots O2W^{ii}$ | 0.89 (3) | 1.93 (3) | 2.824 (2) | 175 (3) |
| $O1W-H1W \cdots N5$ | 0.81 (3) | 2.24 (3) | 2.982 (2) | 153 (3) |
| $N6-H6N \cdots O1W^{iii}$ | 0.84 (2) | 2.07 (2) | 2.905 (2) | 177 (2) |
| $N4-H42 \cdots O1W^{iii}$ | 0.88 (2) | 2.14 (3) | 2.995 (2) | 165 (2) |
| $N4-H41 \cdots O1^{iv}$ | 0.81 (2) | 2.08 (2) | 2.874 (2) | 169 (2) |
| $N3-H32 \cdots N5$ | 0.86 (2) | 2.18 (2) | 2.791 (2) | 128 (2) |
| $N3-H31 \cdots O2W^v$ | 0.83 (2) | 2.27 (2) | 3.082 (2) | 163 (2) |

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

Data collection: SMART (Bruker, 2001); cell refinement: SAINT (Bruker, 2001); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL (Sheldrick, 2008); software used to prepare material for publication: SHELXTL.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI5086).

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supplementary materials

Acta Cryst. (2010). E66, o1209-o1210 [doi:10.1107/S1600536810015357]

N'-Acetyl-5-amino-1-methyl-1*H*-pyrazole-4-carbohydrazonamide dihydrate

A. V. Dolzhenko, A. V. Dolzhenko, G. K. Tan, L. L. Koh and G. Pastorin

Comment

Pyrazoles have been well recognized as valuable ligands in metal-organic chemistry (Mukherjee, 2000; Halcrow, 2009). Pyrazoles also possess useful agricultural (Lamberth, 2007) and pharmacological (Elguero *et al.*, 2002) properties and serve as synthons for other pyrazolo fused bioactive heterocycles (Schenone *et al.*, 2007; Dolzhenko *et al.*, 2008).

Herein, we report molecular and crystal structure of *N'*-acetyl-5-amino-1-methyl-1*H*-pyrazole-4-carbohydrazonamide (Figs. 1 and 2). The compound can exist in two tautomeric forms, namely hydrazonamide and imidohydrazide (Fig. 3). The hydrazonamide tautomer can also exhibit (*E-Z*) isomerism by inversion of configuration of the hydrazono C=N linkage. We found that the compound crystallizes as a *N'*-acetyl-5-amino-1-methyl-1*H*-pyrazole-4-carbohydrazonamide tautomer. Similarly to previously reported *N'*-acetyl-2-phenylethanehydrazonamide (Ianelli *et al.*, 2001), the hydrazonamide group of *N'*-acetyl-5-amino-1-methyl-1*H*-pyrazole-4-carbohydrazonamide adopts (*Z*)-configuration. This configuration is stabilized by the intramolecular N(3)H \cdots N5=C5 hydrogen bonding between the amino group and the hydrazone N5 atom, generating an *S*(6) graph-set motif (Bernstein *et al.*, 1995). Similar NH \cdots O=C interactions were reported for the structurally related derivatives of 5-amino-1*H*-pyrazole-4-carboxylic acid (Zia-ur-Rehman *et al.*, 2008; Zia-ur-Rehman *et al.*, 2009; Caruso *et al.*, 2009). Planarity of the molecule is affected by slight twisting of the acetyl group [C5—N5—N6—C6 torsion angle is 170.14 (16) $^\circ$].

In the crystal, the hydrazonamide molecules are arranged to form sheets parallel to the ($\bar{1}01$) (Fig. 2). In the sheets, atom N4 of one molecule is involved in a intermolecular N—H \cdots O=C interaction with the carbonyl atom O1 of adjacent molecule making *C*(7) chains along the [010] direction. The water molecules further stabilize packing by formation of the intermolecular hydrogen bond network (Fig. 2 and Table 1).

Experimental

N'-Acetyl-5-amino-1-methyl-1*H*-pyrazole-4-carbohydrazonamide was prepared by treatment of ethyl *N*-(4-cyano-1-methyl-1*H*-pyrazol-5-yl)acetimidate with 3 eq. of hydrazine hydrate (40%) in ethanol. Detail procedure with proposed mechanism will be reported elsewhere. Single crystals suitable for the crystallographic analysis were grown by recrystallization from ethanol, m.p. 513 K.

Refinement

All C-bound H atoms were positioned geometrically and included in the refinement in riding-motion approximation [0.95 Å for C_{pyrazole}-H, and 0.98 Å for methyl groups; U_{iso}(H) = 1.2U_{eq}(C_{pyrazole}) and U_{iso}(H) = 1.5U_{eq}(C_{methyl})] while the N- and O-bound H atoms were located in a difference map and refined freely.

Figures

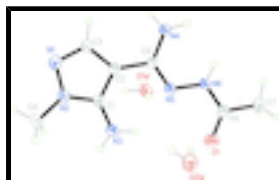


Fig. 1. The molecular structure of *N'*-acetyl-5-amino-1-methyl-1*H*-pyrazole-4-carbohydrazonamide dihydrate showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

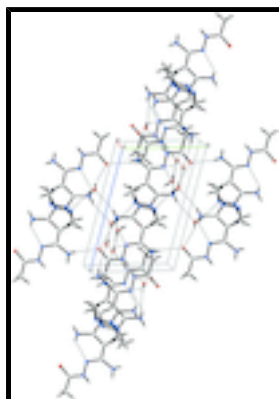


Fig. 2. Crystal packing of the title compound, viewed along the *a* axis.



Fig. 3. Hydrazonamide-imido-hydrazone tautomerism in *N'*-acetyl-5-amino-1-methyl-1*H*-pyrazole-4-carbohydrazonamide

***N'*-Acetyl-5-amino-1-methyl-1*H*-pyrazole-4-carbohydrazonamide dihydrate**

Crystal data

$C_7H_{12}N_6O \cdot 2H_2O$

$M_r = 232.26$

Triclinic, $P\bar{1}$

Hall symbol: -P 1

$a = 7.5496$ (9) Å

$b = 7.6208$ (9) Å

$c = 11.2518$ (13) Å

$\alpha = 102.645$ (2)°

$\beta = 101.440$ (2)°

$\gamma = 110.810$ (2)°

$V = 562.75$ (11) Å³

$Z = 2$

$F(000) = 248$

$D_x = 1.371$ Mg m⁻³

Melting point: 513 K

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

Cell parameters from 1515 reflections

$\theta = 3.0$ – 27.5 °

$\mu = 0.11$ mm⁻¹

$T = 223$ K

Rod, colourless

$0.45 \times 0.12 \times 0.10$ mm

Data collection

Bruker SMART APEX CCD diffractometer

Radiation source: fine-focus sealed tube graphite

φ and ω scans

Absorption correction: multi-scan

2548 independent reflections

2174 reflections with $I > 2\sigma(I)$

$R_{int} = 0.021$

$\theta_{max} = 27.5$ °, $\theta_{min} = 3.0$ °

$h = -9 \rightarrow 9$

(SADABS; Sheldrick, 2001)

$T_{\min} = 0.953$, $T_{\max} = 0.989$

3963 measured reflections

$k = -9 \rightarrow 9$

$l = -14 \rightarrow 13$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.052$

$wR(F^2) = 0.141$

$S = 1.05$

2548 reflections

183 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

$w = 1/[\sigma^2(F_o^2) + (0.0711P)^2 + 0.1961P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 0.31 \text{ e } \text{\AA}^{-3}$

$\Delta\rho_{\min} = -0.25 \text{ e } \text{\AA}^{-3}$

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.

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 $F^2 > 2\sigma(F^2)$ 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 | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|------------|--------------|--------------|----------------------------------|
| O1 | 0.3615 (2) | 0.89463 (19) | 0.14623 (12) | 0.0421 (4) |
| N1 | 0.7337 (2) | 0.3950 (2) | 0.48625 (14) | 0.0306 (4) |
| N2 | 0.7791 (2) | 0.5933 (2) | 0.51428 (13) | 0.0264 (3) |
| N3 | 0.7066 (3) | 0.8221 (2) | 0.42298 (16) | 0.0302 (4) |
| H31 | 0.748 (3) | 0.907 (3) | 0.495 (2) | 0.036 (6)* |
| H32 | 0.613 (3) | 0.821 (3) | 0.365 (2) | 0.039 (6)* |
| N4 | 0.3308 (2) | 0.2471 (2) | 0.11287 (15) | 0.0297 (4) |
| H41 | 0.350 (3) | 0.158 (3) | 0.132 (2) | 0.032 (5)* |
| H42 | 0.260 (3) | 0.223 (3) | 0.034 (2) | 0.040 (6)* |
| N5 | 0.4378 (2) | 0.5945 (2) | 0.18078 (13) | 0.0294 (4) |
| N6 | 0.3198 (2) | 0.5816 (2) | 0.06398 (13) | 0.0267 (3) |
| H6N | 0.269 (3) | 0.479 (3) | 0.000 (2) | 0.037 (6)* |
| C1 | 0.6808 (2) | 0.6344 (2) | 0.41838 (15) | 0.0239 (4) |
| C2 | 0.5664 (2) | 0.4541 (2) | 0.32050 (15) | 0.0236 (4) |

supplementary materials

| | | | | |
|-----|------------|------------|---------------|------------|
| C3 | 0.6068 (3) | 0.3143 (3) | 0.37018 (16) | 0.0272 (4) |
| H3 | 0.5496 | 0.1780 | 0.3256 | 0.033* |
| C4 | 0.9204 (3) | 0.7328 (3) | 0.63443 (17) | 0.0359 (4) |
| H4A | 1.0140 | 0.8443 | 0.6188 | 0.054* |
| H4C | 0.9916 | 0.6687 | 0.6766 | 0.054* |
| H4D | 0.8504 | 0.7791 | 0.6886 | 0.054* |
| C5 | 0.4374 (2) | 0.4304 (2) | 0.19753 (15) | 0.0225 (3) |
| C6 | 0.2965 (3) | 0.7431 (3) | 0.05365 (16) | 0.0278 (4) |
| C7 | 0.1873 (3) | 0.7318 (3) | -0.07661 (17) | 0.0354 (4) |
| H7A | 0.0729 | 0.7603 | -0.0721 | 0.053* |
| H7B | 0.1431 | 0.6000 | -0.1353 | 0.053* |
| H7C | 0.2751 | 0.8278 | -0.1066 | 0.053* |
| O1W | 0.8443 (2) | 0.7733 (2) | 0.15574 (13) | 0.0380 (4) |
| H1W | 0.752 (5) | 0.757 (4) | 0.186 (3) | 0.069 (9)* |
| H2W | 0.949 (5) | 0.780 (4) | 0.213 (3) | 0.065 (8)* |
| O2W | 0.1806 (2) | 0.8169 (2) | 0.34309 (14) | 0.0393 (4) |
| H3W | 0.253 (4) | 0.812 (4) | 0.294 (3) | 0.064 (9)* |
| H4W | 0.189 (4) | 0.731 (4) | 0.381 (3) | 0.060 (8)* |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|-------------|-------------|------------|------------|-------------|------------|
| O1 | 0.0739 (10) | 0.0235 (7) | 0.0262 (7) | 0.0259 (7) | 0.0028 (7) | 0.0046 (5) |
| N1 | 0.0382 (8) | 0.0292 (8) | 0.0260 (8) | 0.0170 (7) | 0.0052 (6) | 0.0107 (6) |
| N2 | 0.0311 (7) | 0.0255 (7) | 0.0195 (7) | 0.0118 (6) | 0.0023 (6) | 0.0060 (6) |
| N3 | 0.0413 (9) | 0.0219 (7) | 0.0218 (8) | 0.0130 (7) | 0.0021 (7) | 0.0032 (6) |
| N4 | 0.0436 (9) | 0.0173 (7) | 0.0228 (8) | 0.0136 (6) | -0.0018 (6) | 0.0053 (6) |
| N5 | 0.0403 (8) | 0.0219 (7) | 0.0197 (7) | 0.0141 (6) | -0.0034 (6) | 0.0043 (6) |
| N6 | 0.0375 (8) | 0.0195 (7) | 0.0174 (7) | 0.0128 (6) | -0.0022 (6) | 0.0029 (6) |
| C1 | 0.0268 (8) | 0.0265 (8) | 0.0186 (7) | 0.0119 (7) | 0.0058 (6) | 0.0071 (6) |
| C2 | 0.0286 (8) | 0.0225 (8) | 0.0199 (8) | 0.0119 (6) | 0.0046 (6) | 0.0072 (6) |
| C3 | 0.0342 (9) | 0.0228 (8) | 0.0241 (8) | 0.0138 (7) | 0.0037 (7) | 0.0076 (6) |
| C4 | 0.0374 (10) | 0.0406 (11) | 0.0206 (8) | 0.0142 (8) | -0.0003 (7) | 0.0043 (8) |
| C5 | 0.0274 (8) | 0.0211 (8) | 0.0188 (7) | 0.0114 (6) | 0.0045 (6) | 0.0061 (6) |
| C6 | 0.0353 (9) | 0.0264 (8) | 0.0217 (8) | 0.0143 (7) | 0.0048 (7) | 0.0085 (7) |
| C7 | 0.0447 (11) | 0.0370 (10) | 0.0273 (9) | 0.0227 (9) | 0.0026 (8) | 0.0136 (8) |
| O1W | 0.0406 (8) | 0.0395 (8) | 0.0236 (7) | 0.0125 (6) | 0.0021 (6) | 0.0044 (6) |
| O2W | 0.0518 (9) | 0.0414 (8) | 0.0299 (7) | 0.0253 (7) | 0.0082 (7) | 0.0145 (6) |

Geometric parameters (\AA , $^\circ$)

| | | | |
|--------|-----------|--------|-----------|
| O1—C6 | 1.236 (2) | C1—C2 | 1.401 (2) |
| N1—C3 | 1.317 (2) | C2—C3 | 1.402 (2) |
| N1—N2 | 1.372 (2) | C2—C5 | 1.459 (2) |
| N2—C1 | 1.344 (2) | C3—H3 | 0.94 |
| N2—C4 | 1.445 (2) | C4—H4A | 0.97 |
| N3—C1 | 1.362 (2) | C4—H4C | 0.97 |
| N3—H31 | 0.83 (2) | C4—H4D | 0.97 |
| N3—H32 | 0.86 (2) | C6—C7 | 1.500 (2) |

| | | | |
|-------------|--------------|-------------|--------------|
| N4—C5 | 1.350 (2) | C7—H7A | 0.97 |
| N4—H41 | 0.81 (2) | C7—H7B | 0.97 |
| N4—H42 | 0.88 (2) | C7—H7C | 0.97 |
| N5—C5 | 1.303 (2) | O1W—H1W | 0.81 (3) |
| N5—N6 | 1.3953 (19) | O1W—H2W | 0.89 (3) |
| N6—C6 | 1.330 (2) | O2W—H3W | 0.86 (3) |
| N6—H6N | 0.84 (2) | O2W—H4W | 0.87 (3) |
| C3—N1—N2 | 104.63 (14) | C2—C3—H3 | 123.7 |
| C1—N2—N1 | 112.10 (14) | N2—C4—H4A | 109.5 |
| C1—N2—C4 | 127.04 (15) | N2—C4—H4C | 109.5 |
| N1—N2—C4 | 120.85 (14) | H4A—C4—H4C | 109.5 |
| C1—N3—H31 | 117.5 (15) | N2—C4—H4D | 109.5 |
| C1—N3—H32 | 110.8 (16) | H4A—C4—H4D | 109.5 |
| H31—N3—H32 | 119 (2) | H4C—C4—H4D | 109.5 |
| C5—N4—H41 | 116.7 (15) | N5—C5—N4 | 126.14 (15) |
| C5—N4—H42 | 123.9 (15) | N5—C5—C2 | 114.92 (14) |
| H41—N4—H42 | 118 (2) | N4—C5—C2 | 118.95 (15) |
| C5—N5—N6 | 117.52 (14) | O1—C6—N6 | 121.90 (15) |
| C6—N6—N5 | 117.50 (14) | O1—C6—C7 | 121.68 (16) |
| C6—N6—H6N | 119.6 (15) | N6—C6—C7 | 116.42 (15) |
| N5—N6—H6N | 122.8 (15) | C6—C7—H7A | 109.5 |
| N2—C1—N3 | 122.61 (15) | C6—C7—H7B | 109.5 |
| N2—C1—C2 | 106.59 (14) | H7A—C7—H7B | 109.5 |
| N3—C1—C2 | 130.72 (15) | C6—C7—H7C | 109.5 |
| C1—C2—C3 | 104.15 (14) | H7A—C7—H7C | 109.5 |
| C1—C2—C5 | 125.02 (15) | H7B—C7—H7C | 109.5 |
| C3—C2—C5 | 130.83 (15) | H1W—O1W—H2W | 110 (3) |
| N1—C3—C2 | 112.53 (15) | H3W—O2W—H4W | 103 (3) |
| N1—C3—H3 | 123.7 | | |
| C3—N1—N2—C1 | 0.66 (19) | N2—N1—C3—C2 | -0.1 (2) |
| C3—N1—N2—C4 | -178.36 (16) | C1—C2—C3—N1 | -0.5 (2) |
| C5—N5—N6—C6 | 170.14 (16) | C5—C2—C3—N1 | 179.83 (17) |
| N1—N2—C1—N3 | -177.99 (15) | N6—N5—C5—N4 | -1.0 (3) |
| C4—N2—C1—N3 | 1.0 (3) | N6—N5—C5—C2 | 178.89 (14) |
| N1—N2—C1—C2 | -0.95 (19) | C1—C2—C5—N5 | 1.9 (2) |
| C4—N2—C1—C2 | 178.00 (16) | C3—C2—C5—N5 | -178.43 (17) |
| N2—C1—C2—C3 | 0.82 (18) | C1—C2—C5—N4 | -178.18 (16) |
| N3—C1—C2—C3 | 177.53 (18) | C3—C2—C5—N4 | 1.5 (3) |
| N2—C1—C2—C5 | -179.44 (15) | N5—N6—C6—O1 | -6.2 (3) |
| N3—C1—C2—C5 | -2.7 (3) | N5—N6—C6—C7 | 173.75 (16) |

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> |
|------------------------------------|-------------|---------------------|----------------------------|-------------------------------|
| O2W—H4W \cdots N1 ⁱ | 0.87 (3) | 2.04 (3) | 2.884 (2) | 162 (3) |
| O2W—H3W \cdots O1 | 0.86 (3) | 2.11 (3) | 2.885 (2) | 150 (3) |
| O1W—H2W \cdots O2W ⁱⁱ | 0.89 (3) | 1.93 (3) | 2.824 (2) | 175 (3) |
| O1W—H1W \cdots N5 | 0.81 (3) | 2.24 (3) | 2.982 (2) | 153 (3) |

supplementary materials

| | | | | |
|-----------------------------|----------|----------|-----------|---------|
| N6—H6N···O1W ⁱⁱⁱ | 0.84 (2) | 2.07 (2) | 2.905 (2) | 177 (2) |
| N4—H42···O1W ⁱⁱⁱ | 0.88 (2) | 2.14 (3) | 2.995 (2) | 165 (2) |
| N4—H41···O1 ^{iv} | 0.81 (2) | 2.08 (2) | 2.874 (2) | 169 (2) |
| N3—H32···N5 | 0.86 (2) | 2.18 (2) | 2.791 (2) | 128 (2) |
| N3—H31···O2W ^v | 0.83 (2) | 2.27 (2) | 3.082 (2) | 163 (2) |

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

Fig. 1

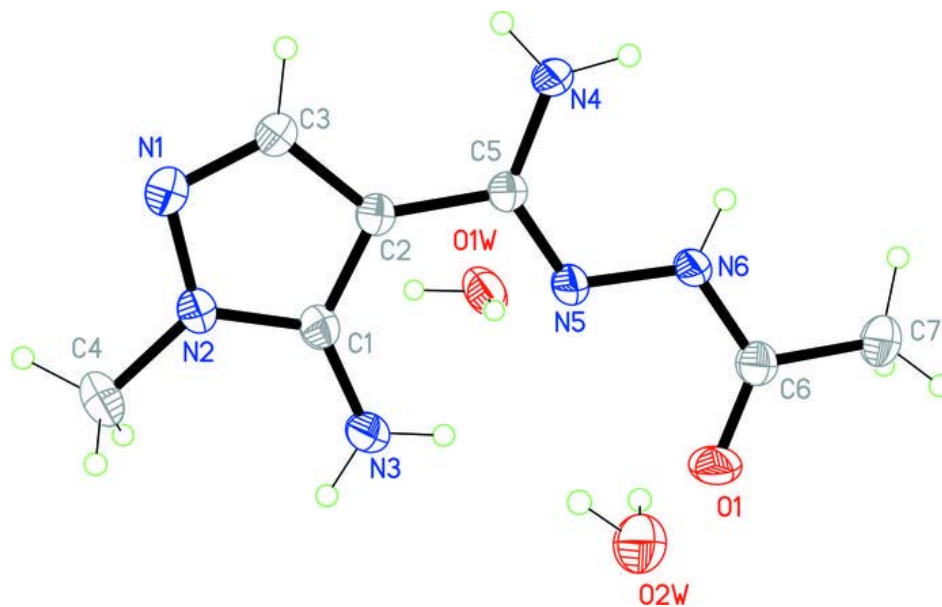


Fig. 2

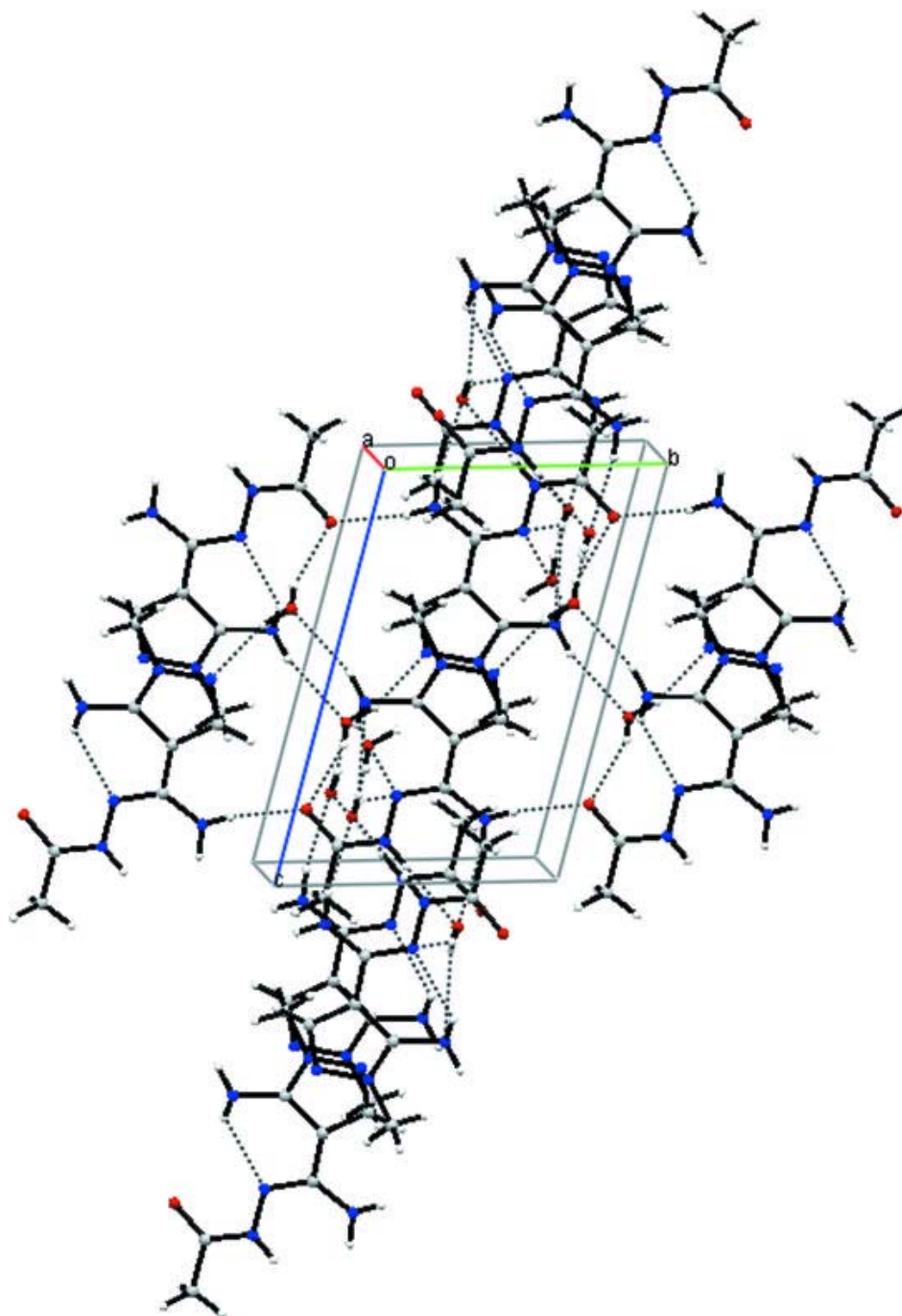


Fig. 3

