Hydrogen bonding in the crystal structure of the molecular salt of pyrazole–pyrazolium picrate

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The asymmetric unit of the title organic salt [systematic name: $1H$-pyrazol-2-ium 2,4,6-trinitrophenolate–$1H$-pyrazole (1/1)], $H(C_3H_4N_2)_2^+ \cdot C_6H_2N_3O_7^-$, consists of one picrate anion and one hydrogen-bonded dimer of a pyrazolium monocation. The H atom involved in the dimer N—H···N hydrogen bond is disordered over both symmetry-unique pyrazole molecules with occupancies of 0.52 (5) and 0.48 (5). In the crystal, the component ions are linked into chains along [100] by two different bifurcated N—H···(O,O) hydrogen bonds. In addition, weak C—H···O hydrogen bonds link inversion-related chains, forming columns along [100].

1. Chemical context

Research interest on co-crystals or organic complex salts in recent years has been prompted by their potential utilization in the pharmaceutical industry (Blagden *et al.*, 2014; Duggirala *et al.*, 2016). Imidazole and pyrazole derivatives are often used as co-crystallized pharmaceutical ingredients (Shimpi *et al.*, 2014). Our investigations involve studies of weak intermolecular interactions in co-crystallized compounds. As part of our continuing study on organic salts formed by imidazole derivatives and picric acid (Song *et al.*, 2016; Su *et al.*, 2008), we report herein the crystal structure of the title compound (I).
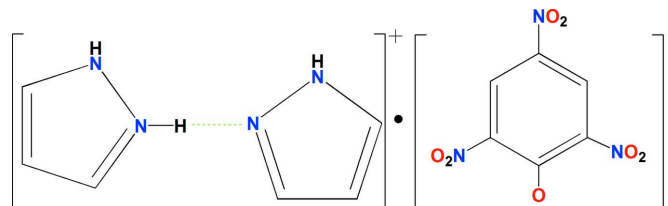
2. Structural commentary

The asymmetric unit of the title compound is shown in Fig. 1. It consists of one picrate anion and two pyrazole molecules, which are connected by an N—H···N hydrogen bond (Table 1), forming a dimeric pyrazolium monocation. The H atom of the hydrogen bond is disordered over both pyrazole molecules. In the dimeric monocation, the two pyrazole rings form a dihedral angle of 74.6 (1)°. In the anion, the C—O_{phenol} bond [1.257 (3)Å] is shorter by *ca* 0.05Å than an average C—O single bond in a neutral picric acid molecule [1.308 (2)Å] calculated statistically by analysis of a CSD search (Groom *et al.*, 2016; Allen, 2002). The C1—C2 [1.438 (4)Å] and C1—C6 [1.449 (4)Å] bonds are significantly longer than the other four benzene C-C bonds [1.367 (4)–1.380 (4)Å]. The C2—C1—C6
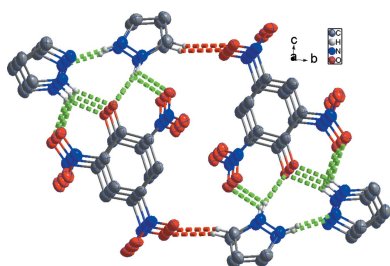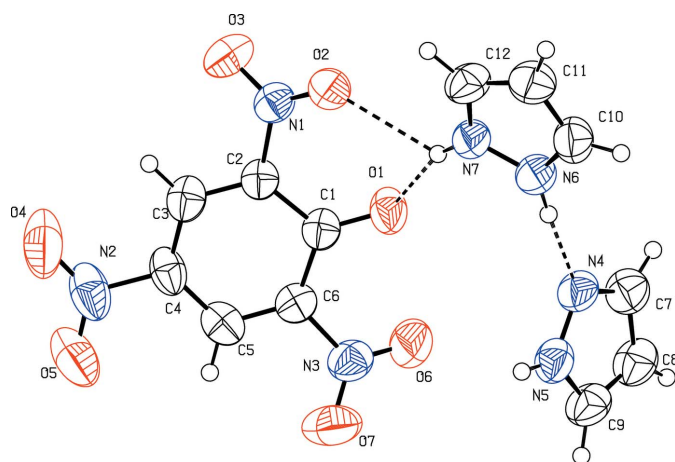
Figure 1
The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. Hydrogen bonds are shown as dashed lines. Only one orientation of the disordered N—H···N hydrogen bond is shown.

[111.9 (2)°] angle is smaller than the ideal value of 120° for a regular hexagon and the other five benzene inner angles of 119.0 (3)–124.4 (3). All variations of bond lengths and angles demonstrate that the negative charge on the phenol oxygen atom is delocalized over the aromatic ring, giving double-bond character for the C1—O1 bond due to the electron-withdrawing effect of the three nitro groups. This is similar to what is observed in some picrate-containing analogs (Zakharov *et al.*, 2015; Gomathi & Kalaivani, 2015). The mean planes of the nitro groups in the anion, are twisted from the benzene ring by dihedral angles of 30.8 (2), 4.8 (3)° and 27.2 (4)° for N1/O2/O3, N2/O4/O5 and N3/O6/O7, respectively. The two *ortho*-nitro groups are twisted out of the benzene ring to a greater extent than the *para*-nitro group. This is most likely due to the steric hindrance between the *ortho*-nitro groups and the phenolic oxygen atom.

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

D—H···A	D—H	H···A	D···A	D—H···A
N4—H4A···N6	0.86 (1)	1.81 (1)	2.663 (3)	173 (7)
N5—H5A···O1[i]	0.87 (1)	1.95 (1)	2.789 (3)	163 (3)
N5—H5A···O6[i]	0.87 (1)	2.42 (3)	2.961 (4)	121 (3)
N6—H6A···N4	0.86 (1)	1.81 (1)	2.663 (3)	174 (7)
N7—H7A···O1	0.86 (1)	2.04 (2)	2.864 (3)	160 (3)
N7—H7A···O2	0.86 (1)	2.29 (3)	2.841 (3)	122 (3)
C12—H12···O4[ii]	0.93	2.61	3.512 (5)	165

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

3. Supramolecular features

In the crystal of (I), the component ions are linked into a chain along [100] by N—H···O hydrogen bonds (Table 1, Fig. 2). In addition, inversion-related chains are connected by a weak C12—H12···O4 ($-x, -y + 2, -z + 1$) hydrogen bond, forming columns along [100]. A short O3$_{(nitro)}$···O3$_{(nitro)}$ ($-1 - x, 2 - y, 1 - z$) distance of 2.913 (2) Å is also observed (Spek, 2009). Although the benzene and pyrazolium rings are stacked in a parallel fashion, no significant π–π interactions exist between them (Janiak, 2000). This could be attributed to the deficient π-electron nature resulting from the electron-withdrawing effects of the nitro groups.

4. Database survey

A search of the Cambridge Structural Database (CSD Version 5.37 plus one update; Groom *et al.*, 2016) indicates there are some analogs prepared from picric acid and pyrazole derivatives, *viz.* SASKII, SASLAB, SASKUU, SASLUB (Singh *et al.*, 2012) and SASKII01 (Dhanabal *et al.*, 2013). A similar solvated organic adduct, $C_5H_9N_2^+ \cdot C_6H_2N_3O_7^-$ (SASKII; Singh *et al.*, 2012) indicates that the solvent used for the crystallization process can affect the final product in which the ratio of component ions are different.

5. Synthesis and crystallization

Pyrazole (20.0 mmol, 136.0 mg) and picric acid (10. 0 mmol, 230.0mg) were dissolved in a 2:1 molar ratio in 95% methanol (50.0 ml). The mixture was stirred for an hour at 323 K and then cooled to room temperature and filtered. The resulting yellow solution was kept in air for two weeks. Needle-like yellow crystals of (I) suitable for single-crystal X-ray diffraction analysis were grown by slow evaporation of the solution. The crystals were separated by filtration (yield, 60%, *ca* 0.22 g).

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. H atoms bonded to C atoms were positioned geometrically with C—H = 0.93 Å (aromatic) and refined in a riding-model approximation with $U_{iso}(H) = 1.2U_{eq}(C)$. H atoms bonded to N atoms were refined with a

Figure 2
Part of the crystal structure of (I), showing the formation of hydrogen-bonded columns along [100]. For clarity, H atoms not involved in the motif have been omitted. Green and red dashed lines indicate the N—H···O hydrogen bonds and weak C—H···O hydrogen bonds, respectively.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_3H_5N_2{}^+ \cdot C_6H_2N_3O_7{}^- \cdot C_3H_4N_2$
M_r	365.28
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	298
a, b, c (Å)	4.2447 (14), 16.950 (5), 21.839 (7)
β (°)	92.029 (6)
V (Å^3)	1570.3 (9)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.13
Crystal size (mm)	$0.45 \times 0.06 \times 0.04$
Data collection	
Diffractometer	Bruker SMART CCD
Absorption correction	Multi-scan (SADABS; Sheldrick, 1996)
T_{min}, T_{max}	0.736, 0.875
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	12038, 3086, 1787
R_{int}	0.050
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.617
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.057, 0.157, 0.98
No. of reflections	3086
No. of parameters	248
No. of restraints	4
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å^{-3})	0.18, −0.16

Computer programs: *SMART* and *SAINT* (Bruker, 2001), *SHELXS* and *SHELXTL* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015) and *DIAMOND* (Brandenburg, 2006).

constraint of d_{N-H} = 0.86 (1) Å and $U_{iso}(H)$ = 1.2$U_{eq}(N)$. Atoms H4A and H6A were found in difference Fourier maps and refined as disordered using the PART command (Sheldrick, 2015). The final site occupancies of the two hydrogen-atom components were 0.52 (1):0.48 (1) for H6A and H4A, respectively.

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Computing details

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT* (Bruker, 2001); program(s) used to solve structure: *SHELXS* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *SHELXTL* (Sheldrick, 2008) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

1*H*-Pyrazol-2-ium 2,4,6-trinitrophenolate 1*H*-pyrazole

Crystal data

$C_3H_5N_2^+ \cdot C_6H_2N_3O_7^- \cdot C_3H_4N_2$	$F(000) = 752$
$M_r = 365.28$	$D_x = 1.545$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 4.2447\,(14)$ Å	Cell parameters from 1735 reflections
$b = 16.950\,(5)$ Å	$\theta = 2.4–20.5°$
$c = 21.839\,(7)$ Å	$\mu = 0.13$ mm^{-1}
$\beta = 92.029\,(6)°$	$T = 298$ K
$V = 1570.3\,(9)$ Å^3	Needle, yellow
$Z = 4$	$0.45 \times 0.06 \times 0.04$ mm

Data collection

Bruker SMART CCD diffractometer	3086 independent reflections
	1787 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.050$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$\theta_{max} = 26.0°$, $\theta_{min} = 1.5°$
	$h = -5 \rightarrow 5$
$T_{min} = 0.736$, $T_{max} = 0.875$	$k = -20 \rightarrow 20$
12038 measured reflections	$l = -26 \rightarrow 24$

Refinement

Refinement on F^2	H atoms treated by a mixture of independent and constrained refinement
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.057$	$w = 1/[\sigma^2(F_o^2) + (0.0698P)^2 + 0.3803P]$
$wR(F^2) = 0.157$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.98$	$(\Delta/\sigma)_{max} < 0.001$
3086 reflections	$\Delta\rho_{max} = 0.18$ e Å^{-3}
248 parameters	$\Delta\rho_{min} = -0.16$ e Å^{-3}
4 restraints	

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_{iso}*/U_{eq}	Occ. (<1)
C1	0.2577 (7)	0.78567 (15)	0.50270 (13)	0.0502 (7)	
C2	0.0904 (7)	0.85715 (15)	0.51570 (12)	0.0478 (7)	
C3	0.0496 (7)	0.88621 (16)	0.57336 (13)	0.0565 (8)	
H3	−0.0667	0.9320	0.5789	0.068*	
C4	0.1825 (8)	0.84691 (17)	0.62309 (13)	0.0577 (8)	
C5	0.3503 (7)	0.77808 (17)	0.61557 (13)	0.0573 (8)	
H5	0.4423	0.7525	0.6494	0.069*	
C6	0.3802 (7)	0.74780 (15)	0.55807 (13)	0.0506 (7)	
C7	0.7321 (8)	0.56590 (19)	0.33757 (15)	0.0683 (9)	
H7	0.5902	0.5601	0.3045	0.082*	
C8	0.8600 (8)	0.50504 (18)	0.37140 (16)	0.0689 (9)	
H8	0.8229	0.4514	0.3660	0.083*	
C9	1.0517 (8)	0.53966 (19)	0.41426 (15)	0.0679 (9)	
H9	1.1731	0.5137	0.4443	0.082*	
C10	0.8031 (8)	0.80992 (19)	0.26399 (14)	0.0675 (9)	
H10	0.9374	0.7862	0.2367	0.081*	
C11	0.6789 (9)	0.88402 (19)	0.25746 (15)	0.0698 (9)	
H11	0.7114	0.9197	0.2260	0.084*	
C12	0.4981 (8)	0.89415 (18)	0.30687 (15)	0.0648 (9)	
H12	0.3809	0.9388	0.3157	0.078*	
N1	−0.0457 (6)	0.90430 (13)	0.46540 (12)	0.0532 (6)	
N2	0.1422 (9)	0.87879 (19)	0.68408 (13)	0.0815 (9)	
N3	0.5497 (7)	0.67352 (16)	0.55396 (14)	0.0645 (7)	
N4	0.8395 (7)	0.63381 (15)	0.35881 (12)	0.0613 (7)	
H4A	0.808 (16)	0.6815 (15)	0.346 (3)	0.074*	0.48 (5)
N5	1.0360 (7)	0.61758 (14)	0.40591 (12)	0.0617 (7)	
H5A	1.133 (7)	0.6554 (14)	0.4254 (13)	0.074*	
N6	0.7043 (7)	0.77681 (14)	0.31469 (12)	0.0600 (7)	
H6A	0.761 (15)	0.7321 (19)	0.330 (3)	0.072*	0.52 (5)
N7	0.5183 (6)	0.82915 (14)	0.34019 (11)	0.0553 (6)	
H7A	0.434 (7)	0.8196 (18)	0.3747 (8)	0.066*	
O1	0.2919 (6)	0.75921 (11)	0.44959 (9)	0.0668 (6)	
O2	0.0820 (5)	0.90477 (13)	0.41655 (9)	0.0709 (7)	
O3	−0.2780 (5)	0.94352 (13)	0.47569 (11)	0.0756 (7)	
O4	−0.0220 (9)	0.93651 (17)	0.68985 (11)	0.1281 (13)	
O5	0.2766 (8)	0.84518 (17)	0.72727 (12)	0.1047 (10)	
O6	0.4897 (7)	0.62868 (15)	0.51168 (12)	0.0976 (9)	
O7	0.7405 (7)	0.65737 (15)	0.59511 (13)	0.0968 (9)	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0571 (19)	0.0411 (15)	0.0529 (18)	−0.0044 (13)	0.0093 (14)	0.0021 (13)
C2	0.0536 (18)	0.0405 (14)	0.0496 (17)	−0.0054 (13)	0.0070 (14)	0.0018 (12)
C3	0.069 (2)	0.0407 (15)	0.0609 (19)	−0.0060 (14)	0.0160 (16)	0.0012 (14)
C4	0.083 (2)	0.0481 (17)	0.0431 (17)	−0.0152 (16)	0.0113 (16)	−0.0028 (13)
C5	0.067 (2)	0.0531 (17)	0.0517 (18)	−0.0163 (15)	0.0001 (15)	0.0063 (14)
C6	0.0516 (18)	0.0417 (15)	0.0586 (19)	−0.0056 (13)	0.0047 (14)	0.0059 (13)
C7	0.081 (2)	0.0542 (19)	0.070 (2)	0.0002 (17)	0.0032 (18)	0.0008 (16)
C8	0.082 (2)	0.0443 (17)	0.081 (2)	0.0001 (17)	0.011 (2)	0.0028 (17)
C9	0.079 (2)	0.0543 (19)	0.072 (2)	0.0136 (17)	0.0130 (19)	0.0148 (16)
C10	0.082 (2)	0.064 (2)	0.057 (2)	0.0059 (18)	0.0108 (17)	−0.0026 (16)
C11	0.084 (2)	0.062 (2)	0.064 (2)	0.0043 (18)	0.0063 (18)	0.0165 (16)
C12	0.071 (2)	0.0494 (17)	0.074 (2)	0.0102 (15)	0.0029 (18)	0.0093 (16)
N1	0.0543 (16)	0.0428 (13)	0.0625 (17)	−0.0019 (12)	0.0015 (13)	−0.0003 (12)
N2	0.136 (3)	0.0584 (18)	0.0513 (18)	−0.0198 (18)	0.0169 (18)	−0.0022 (15)
N3	0.0695 (19)	0.0586 (16)	0.0659 (18)	0.0079 (14)	0.0087 (15)	0.0137 (15)
N4	0.080 (2)	0.0445 (15)	0.0593 (17)	0.0116 (14)	0.0079 (15)	0.0077 (13)
N5	0.075 (2)	0.0482 (16)	0.0624 (18)	0.0046 (13)	0.0103 (15)	−0.0023 (13)
N6	0.0765 (19)	0.0439 (14)	0.0593 (17)	0.0071 (13)	−0.0008 (14)	0.0020 (13)
N7	0.0655 (17)	0.0490 (14)	0.0513 (15)	0.0082 (12)	0.0033 (12)	0.0009 (12)
O1	0.1065 (18)	0.0453 (11)	0.0493 (13)	0.0069 (11)	0.0120 (12)	0.0007 (9)
O2	0.0857 (17)	0.0755 (15)	0.0519 (14)	0.0201 (12)	0.0063 (12)	0.0082 (11)
O3	0.0627 (15)	0.0675 (14)	0.0969 (18)	0.0187 (12)	0.0090 (13)	0.0079 (12)
O4	0.244 (4)	0.0713 (18)	0.0722 (18)	0.027 (2)	0.046 (2)	−0.0084 (14)
O5	0.153 (3)	0.106 (2)	0.0549 (16)	−0.0167 (19)	−0.0024 (17)	−0.0058 (14)
O6	0.148 (3)	0.0690 (15)	0.0753 (17)	0.0389 (16)	0.0009 (16)	−0.0061 (14)
O7	0.095 (2)	0.0828 (18)	0.111 (2)	0.0201 (15)	−0.0245 (17)	0.0184 (15)

Geometric parameters (Å, º)

C1—O1	1.257 (3)	C10—N6	1.323 (4)
C1—C2	1.438 (4)	C10—C11	1.368 (4)
C1—C6	1.449 (4)	C10—H10	0.9300
C2—C3	1.369 (4)	C11—C12	1.357 (4)
C2—N1	1.461 (4)	C11—H11	0.9300
C3—C4	1.378 (4)	C12—N7	1.321 (4)
C3—H3	0.9300	C12—H12	0.9300
C4—C5	1.380 (4)	N1—O2	1.214 (3)
C4—N2	1.453 (4)	N1—O3	1.216 (3)
C5—C6	1.367 (4)	N2—O4	1.210 (4)
C5—H5	0.9300	N2—O5	1.225 (4)
C6—N3	1.454 (4)	N3—O6	1.216 (3)
C7—N4	1.316 (4)	N3—O7	1.219 (3)
C7—C8	1.370 (4)	N4—N5	1.330 (4)
C7—H7	0.9300	N4—H4A	0.862 (10)
C8—C9	1.352 (5)	N5—H5A	0.865 (10)

C8—H8	0.9300	N6—N7	1.323 (3)
C9—N5	1.335 (4)	N6—H6A	0.861 (10)
C9—H9	0.9300	N7—H7A	0.861 (10)
O1—C1—C2	123.9 (3)	C11—C10—H10	124.9
O1—C1—C6	124.2 (3)	C12—C11—C10	105.1 (3)
C2—C1—C6	111.9 (2)	C12—C11—H11	127.5
C3—C2—C1	124.4 (3)	C10—C11—H11	127.5
C3—C2—N1	115.8 (2)	N7—C12—C11	107.7 (3)
C1—C2—N1	119.8 (2)	N7—C12—H12	126.1
C2—C3—C4	119.3 (3)	C11—C12—H12	126.1
C2—C3—H3	120.3	O2—N1—O3	123.3 (3)
C4—C3—H3	120.3	O2—N1—C2	119.2 (2)
C3—C4—C5	120.9 (3)	O3—N1—C2	117.5 (3)
C3—C4—N2	119.0 (3)	O4—N2—O5	123.3 (3)
C5—C4—N2	120.1 (3)	O4—N2—C4	118.9 (3)
C6—C5—C4	119.5 (3)	O5—N2—C4	117.8 (3)
C6—C5—H5	120.3	O6—N3—O7	122.3 (3)
C4—C5—H5	120.3	O6—N3—C6	119.8 (3)
C5—C6—C1	123.9 (3)	O7—N3—C6	117.8 (3)
C5—C6—N3	116.4 (3)	C7—N4—N5	106.9 (3)
C1—C6—N3	119.7 (3)	C7—N4—H4A	131 (5)
N4—C7—C8	110.1 (3)	N5—N4—H4A	122 (5)
N4—C7—H7	125.0	N4—N5—C9	109.7 (3)
C8—C7—H7	125.0	N4—N5—H5A	120 (2)
C9—C8—C7	105.3 (3)	C9—N5—H5A	130 (2)
C9—C8—H8	127.3	C10—N6—N7	106.2 (2)
C7—C8—H8	127.3	C10—N6—H6A	127 (4)
N5—C9—C8	108.0 (3)	N7—N6—H6A	126 (4)
N5—C9—H9	126.0	C12—N7—N6	110.8 (3)
C8—C9—H9	126.0	C12—N7—H7A	128 (2)
N6—C10—C11	110.2 (3)	N6—N7—H7A	121 (2)
N6—C10—H10	124.9		
O1—C1—C2—C3	179.5 (3)	C10—C11—C12—N7	0.2 (4)
C6—C1—C2—C3	−0.3 (4)	C3—C2—N1—O2	148.3 (3)
O1—C1—C2—N1	−1.3 (4)	C1—C2—N1—O2	−31.0 (4)
C6—C1—C2—N1	179.0 (2)	C3—C2—N1—O3	−29.2 (4)
C1—C2—C3—C4	2.0 (4)	C1—C2—N1—O3	151.5 (3)
N1—C2—C3—C4	−177.3 (2)	C3—C4—N2—O4	4.1 (5)
C2—C3—C4—C5	−1.3 (4)	C5—C4—N2—O4	−175.5 (3)
C2—C3—C4—N2	179.1 (3)	C3—C4—N2—O5	−176.2 (3)
C3—C4—C5—C6	−1.1 (4)	C5—C4—N2—O5	4.2 (5)
N2—C4—C5—C6	178.5 (3)	C5—C6—N3—O6	152.3 (3)
C4—C5—C6—C1	3.1 (4)	C1—C6—N3—O6	−28.5 (4)
C4—C5—C6—N3	−177.7 (3)	C5—C6—N3—O7	−24.9 (4)
O1—C1—C6—C5	178.0 (3)	C1—C6—N3—O7	154.4 (3)
C2—C1—C6—C5	−2.3 (4)	C8—C7—N4—N5	0.1 (4)

O1—C1—C6—N3	−1.3 (4)	C7—N4—N5—C9	−0.1 (3)
C2—C1—C6—N3	178.5 (2)	C8—C9—N5—N4	0.0 (4)
N4—C7—C8—C9	−0.2 (4)	C11—C10—N6—N7	0.2 (4)
C7—C8—C9—N5	0.1 (4)	C11—C12—N7—N6	−0.1 (4)
N6—C10—C11—C12	−0.2 (4)	C10—N6—N7—C12	−0.1 (4)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4—H4*A*···N6	0.86 (1)	1.81 (1)	2.663 (3)	173 (7)
N5—H5*A*···O1[i]	0.87 (1)	1.95 (1)	2.789 (3)	163 (3)
N5—H5*A*···O6[i]	0.87 (1)	2.42 (3)	2.961 (4)	121 (3)
N6—H6*A*···N4	0.86 (1)	1.81 (1)	2.663 (3)	174 (7)
N7—H7*A*···O1	0.86 (1)	2.04 (2)	2.864 (3)	160 (3)
N7—H7*A*···O2	0.86 (1)	2.29 (3)	2.841 (3)	122 (3)
C12—H12···O4[ii]	0.93	2.61	3.512 (5)	165

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