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Crystal structure of 1-phenyl-1*H*-pyrazolo[3,4-*d*]pyrimidin-4(5*H*)-one

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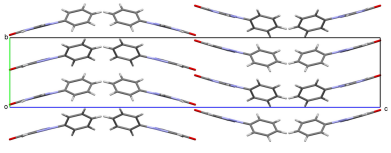
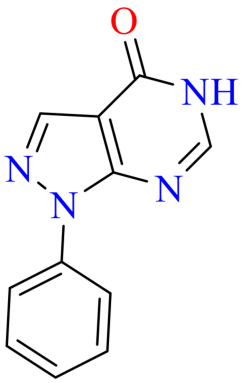
Heating of 5-amino-1-phenyl-1*H*-pyrazole-4-carbonitrile in the presence of formic acid yielded the title compound, $C_{11}H_8N_4O$. The pyrazolo[3,4-*d*]pyrimidine ring system forms a dihedral angle of 34.72 (6)° with the phenyl ring. In the crystal, classical N—H···O and non-classical C—H···O and C—H···N intermolecular interactions result in the formation of supramolecular bands extending parallel to the *a* axis. Additional $\pi\cdots\pi$ interactions between pyrimidine and pyrazole rings, and C—H···π interactions between neighboring phenyl rings consolidate the packing.

1. Chemical context

Cancer is one of the most difficult to treat and rapidly increasing diseases worldwide. The number of cancer types is increasing every year, which worries the World Health Organization and specialists in the field. One of the urgent tasks facing chemists and pharmacists is therefore to create and implement new, effective drugs against cancer. An analysis of the literature shows that pyrazolopyrimidines, a class of compounds we have selected for our research, are among the pharmaceutically active substances. Synthetic pyrazolopyrimidines are widely used in medicine. In particular, drugs based on these compounds are used to repair cells damaged by viruses, microbes, and cancer. Examples of such drugs include allopurinol, istrafilin, and ruxolitinib. Research in the field of pyrazolopyrimidines is advancing with the design, screening, synthesis, and biological evaluation of potential cancer drugs that inhibit tumor growth and induce apoptosis (He *et al.*, 2011; Gillespie *et al.*, 2008; Schenone *et al.*, 2004; Tintori *et al.*, 2015; Gaber *et al.*, 2022; Trivedi *et al.*, 2012). Among these, compounds containing a pyrazolo[3,4-*d*]pyrimidine moiety exhibit broad anticancer activity *in vitro*. These derivatives are of further interest due to their high similarity to the adenine moiety of ATP. To obtain new pyrazolo[3,4-*d*]pyrimidine-4-one derivatives, we carried out the reaction of 5-amino-1-phenyl-1*H*-pyrazole-4-carbonitrile with formic acid, yielding 1-phenyl-1*H*-pyrazolo[3,4-*d*]pyrimidin-4(5*H*)-one, $C_{11}H_8N_4O$, the crystal structure of which is reported here.





2. Structural commentary

The asymmetric unit consist of one formula unit (Fig. 1). Selected N—N and N—C bond lengths given in Table 1 correspond to those observed in related structures [Cambridge Structure Database (CSD; Groom *et al.*, 2016) refcodes CICPAG, NIFGUF, UBAVUS and VICGOD (Yathirajan *et al.*, 2007*a*,*b*; Wang *et al.*, 2021; Ferroni *et al.*, 1990, respectively)]. In the unsubstituted base, 1*H*-pyrazolo-[3,4-*d*]pyrimidin-4(5*H*)-one, the N—N and N—C bond lengths within the pyrazole ring are slightly shorter (N1—N2 = 1.363 Å, N1—C7*A* = 1.343 Å and N2—C3 = 1.313 Å; ALOPUR01, Tang *et al.*, 2023). The pyrazolo[3,4-*d*]pyrimidine ring system is planar with an r.m.s. deviation of 0.012 Å for the ring atoms. The phenyl ring (C8–C13) forms a dihedral angle of 34.72 (6)° with the mean plane of the pyrazolo[3,4-*d*]pyrimidine ring system.

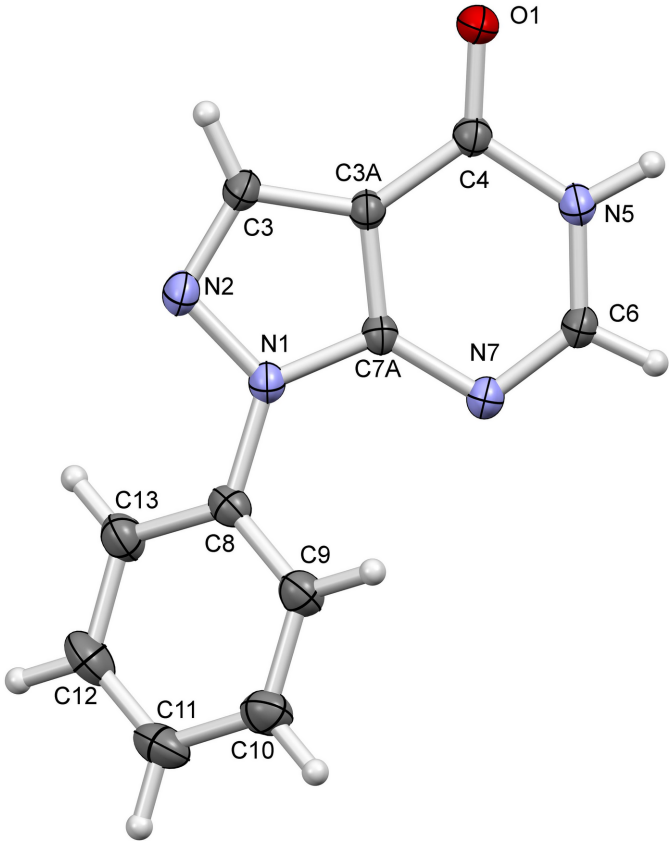


Figure 1
The molecular structure of the title compound, with displacement ellipsoids drawn at the 50% probability level.

Table 1
Selected bond lengths (Å).

N1—C7*A*	1.358 (2)	N2—C3	1.321 (2)
N1—N2	1.376 (2)	N5—C6	1.355 (2)
N1—C8	1.428 (2)	N7—C6	1.304 (2)

Table 2
Hydrogen-bond geometry (Å, °).

*Cg*1 is the centroid of the C8–C13 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N5—H5···O1^{i}	0.94 (3)	1.94 (3)	2.862 (2)	166 (2)
C3—H3···O1^{ii}	0.93	2.28	3.180 (2)	162
C6—H6···N2^{iii}	0.93	2.48	3.374 (2)	162
C9—H9···*Cg*1^{iv}	0.93	2.94	3.767 (2)	150

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

3. Supramolecular features

In the crystal of the title compound, intermolecular N—H···O hydrogen bonds link the molecules into centrosymmetric dimers, forming $R_2^2(8)$ motifs. Other centrosymmetric $R_2^2(10)$ motifs are formed by weak intermolecular C—H···O bonds, and a weak C—H···N hydrogen bond participates in the formation of $R_3^2(8)$ ring motifs (Table 2). These hydrogen bonds generate supramolecular bands running parallel to the *a* axis (Fig. 2). The bands are further packed along the *b*-axis direction through pairs of π–π stacking interactions (Fig. 3)

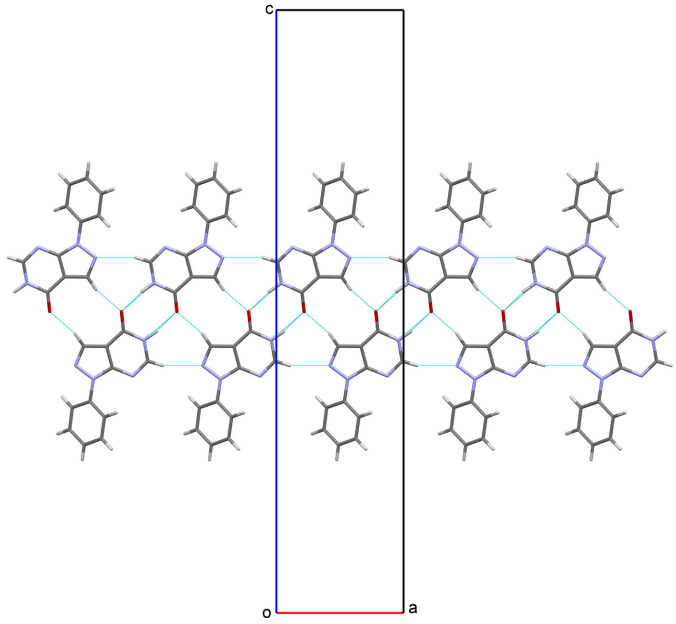


Figure 2
Formation of supramolecular bands running parallel to the *a* axis.

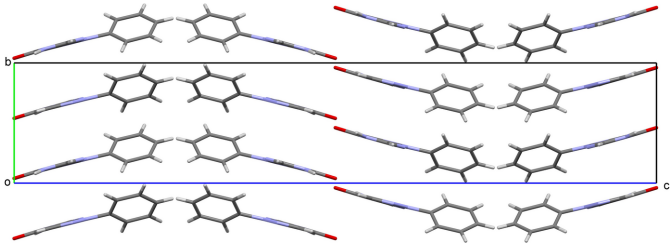


Figure 3
Packing of the supramolecular bands along the *b* axis.

[*Cg*2···*Cg*3^{v} and *Cg*3···*Cg*2^{v}, centroid-to-centroid distances of 3.4644 (11) and 3.6444 (11) Å and a slippage of 0.860 and 1.471 Å, respectively; *Cg*2 is the pyrimidine ring centroid, *Cg*3 is the pyrazole ring centroid; symmetry code: (v) $\frac{3}{2}-x, -\frac{1}{2}+y, z$). In addition, an intermolecular C_{ar}—H···π interaction is observed between the phenyl ring and the centroid of a neighboring phenyl ring (*Cg*1; Table 2).

4. Database survey

A search of the Cambridge Structural Database (CSD; updated 16 May 2025; Groom *et al.*, 2016) revealed 91 relevant entries containing the 1*H*-pyrazolo[3,4-*d*]pyrimidin-4(5*H*)-one moiety. Two of these, namely ALOPUR (Prusiner & Sundaralingam, 1972) and ALOPUR01 (Tang *et al.*, 2023), correspond to allopurinol, *i.e.*, the 1*H*-pyrazolo[3,4-*d*]pyrimidin-4(5*H*)-one structure. Two other entries, SUTRUX and SUTSAE (Dai *et al.*, 2020), are co-crystals of allopurinol. The structures of allopurinol salts with maleic and oxalic acids were determined by powder X-ray diffraction analysis (Varsa *et al.*, 2023). Among the retrieved entries, more than 20 correspond to metal-containing structures.

5. Synthesis and crystallization

The reaction scheme is displayed in Fig. 4. Amino-1-phenyl-1*H*-pyrazole-4-carbonitrile (4. 2 g, 10.8 mmol) was heated in 10 ml of formic acid at 383–385 K for 6 h. Then, the mixture was poured into a 250 ml beaker of ice–water and the resulting precipitate was filtered off and dried. Recrystallization from ethanol yielded 1.98 g (86%) of 1-phenyl-1*H*-pyrazolo[3,4-*d*] pyrimidin-4(5*H*)-one in form of rod-shaped crystals (Fig. 5), m.p. 577–578 K, R_f = 0.38.

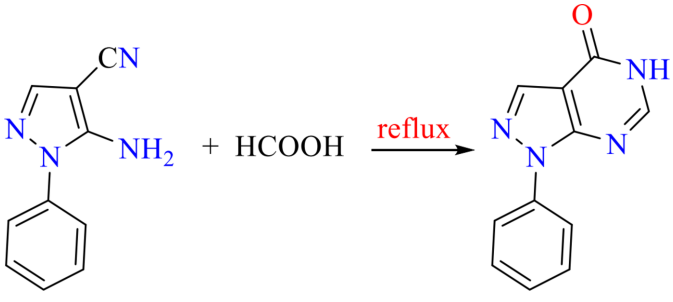


Figure 4
Synthesis scheme for the title compound.

Table 3
Experimental details.

Crystal data	
Chemical formula	$C_{11}H_8N_4O$
M_r	212.21
Crystal system, space group	Orthorhombic, *Pbca*
Temperature (K)	293
a, *b*, *c* (Å)	7.7822 (2), 6.8848 (2), 36.8514 (10)
V (Å^3)	1974.46 (9)
Z	8
Radiation type	Cu *Kα*
μ (mm^{-1})	0.81
Crystal size (mm)	0.44 × 0.12 × 0.05
Data collection	
Diffractometer	Bruker D8 VENTURE dual wavelength Mo/Cu
Absorption correction	Numerical (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.659, 0.753
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	20676, 1807, 1619
R_{int}	0.054
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.602
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.046, 0.120, 1.13
No. of reflections	1807
No. of parameters	150
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.25, −0.19

Computer programs: *APEX5* and *SAINT* (Bruker, 2023), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*), *Mercury* (Macrae *et al.*, 2020) and *publCIF* (Westrip, 2010).

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. Hydrogen atoms bonded to carbon atoms were placed in calculated positions and refined to ride on their parent atoms with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C). The H atom attached to N5 was located in a

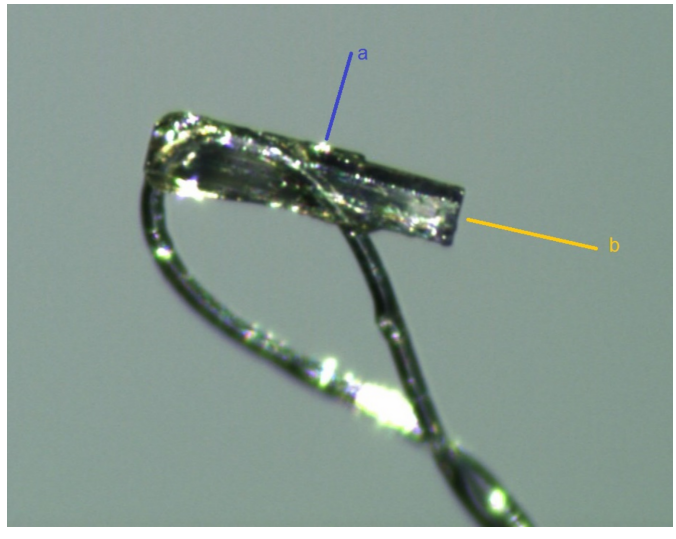


Figure 5
Screenshot from the face-indexing procedure showing the *a* and *b* axes of the rod-shaped crystal.

difference-Fourier map, and its coordinates and isotropic displacement parameter were refined freely.

Acknowledgements

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Crystal structure of 1-phenyl-1*H*-pyrazolo[3,4-*d*]pyrimidin-4(5*H*)-one

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Computing details

1-Phenyl-1*H*-pyrazolo[3,4-*d*]pyrimidin-4(5*H*)-one

Crystal data

$C_{11}H_8N_4O$
M_r = 212.21
Orthorhombic, *Pbca*
a = 7.7822 (2) Å
b = 6.8848 (2) Å
c = 36.8514 (10) Å
V = 1974.46 (9) Å^3
Z = 8
F(000) = 880
D_x = 1.428 Mg m^{-3}
Melting point: 577(2) K
Cu *Kα* radiation, *λ* = 1.54178 Å
Cell parameters from 3849 reflections
θ = 7.2–66.9°
μ = 0.81 mm^{-1}
T = 293 K
Prism, colourless
0.44 × 0.12 × 0.05 mm

Data collection

Bruker D8 VENTURE dual wavelength Mo/Cu diffractometer
Radiation source: microfocus X-ray source, Incoatec I*μ*S 3.0 Microfocus Source
Mirror monochromator
ω–*φ* scans
Absorption correction: numerical (*SADABS*; Krause *et al.*, 2015)
T_{min} = 0.659, T_{max} = 0.753
20676 measured reflections
1807 independent reflections
1619 reflections with $I > 2\sigma(I)$
R_{int} = 0.054
θ_{max} = 68.1°, θ_{min} = 7.2°
h = −9→9
k = −8→8
l = −44→44

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.120
S = 1.13
1807 reflections
150 parameters
0 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0495P)^2 + 0.8037P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}
Extinction correction: SHELXL-2014/7 (Sheldrick 2015b), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0042 (6)

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}
O1	0.78192 (17)	0.5391 (2)	0.49996 (3)	0.0534 (4)
N1	0.56134 (18)	0.6999 (2)	0.38824 (4)	0.0416 (4)
N2	0.42164 (19)	0.6696 (3)	0.41042 (5)	0.0489 (4)
N5	0.9606 (2)	0.6158 (2)	0.45274 (4)	0.0450 (4)
H5	1.056 (3)	0.582 (3)	0.4669 (6)	0.064 (7)*
N7	0.87219 (19)	0.7013 (2)	0.39334 (4)	0.0434 (4)
C3	0.4855 (2)	0.6268 (3)	0.44265 (5)	0.0446 (5)
H3	0.4195	0.5980	0.4630	0.053*
C3A	0.6660 (2)	0.6305 (3)	0.44230 (5)	0.0392 (4)
C4	0.7984 (2)	0.5914 (3)	0.46802 (5)	0.0415 (4)
C6	0.9895 (2)	0.6677 (3)	0.41782 (5)	0.0431 (5)
H6	1.1035	0.6805	0.4106	0.052*
C7A	0.7101 (2)	0.6778 (2)	0.40708 (5)	0.0371 (4)
C8	0.5349 (2)	0.7457 (3)	0.35086 (5)	0.0442 (5)
C9	0.6491 (3)	0.6783 (3)	0.32524 (6)	0.0538 (5)
H9	0.7413	0.6008	0.3321	0.065*
C10	0.6254 (3)	0.7269 (4)	0.28933 (6)	0.0640 (6)
H10	0.7030	0.6827	0.2720	0.077*
C11	0.4895 (4)	0.8388 (4)	0.27881 (7)	0.0696 (7)
H11	0.4747	0.8705	0.2545	0.083*
C12	0.3746 (4)	0.9045 (4)	0.30437 (7)	0.0718 (7)
H12	0.2817	0.9803	0.2972	0.086*
C13	0.3959 (3)	0.8587 (3)	0.34074 (6)	0.0585 (6)
H13	0.3182	0.9031	0.3580	0.070*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0433 (8)	0.0746 (10)	0.0423 (7)	−0.0024 (7)	−0.0020 (6)	0.0144 (6)
N1	0.0323 (8)	0.0477 (9)	0.0448 (9)	0.0009 (6)	−0.0018 (6)	0.0030 (6)
N2	0.0320 (8)	0.0594 (10)	0.0554 (10)	−0.0011 (7)	0.0015 (7)	0.0061 (8)
N5	0.0341 (8)	0.0538 (9)	0.0471 (9)	−0.0006 (7)	−0.0045 (7)	0.0068 (7)
N7	0.0336 (8)	0.0521 (9)	0.0446 (9)	0.0012 (7)	0.0013 (6)	0.0027 (7)
C3	0.0334 (9)	0.0531 (11)	0.0472 (10)	−0.0011 (8)	0.0032 (8)	0.0065 (8)
C3A	0.0331 (9)	0.0417 (9)	0.0427 (10)	0.0002 (7)	−0.0015 (7)	0.0029 (7)
C4	0.0369 (9)	0.0427 (10)	0.0449 (10)	−0.0007 (7)	−0.0004 (7)	0.0028 (7)
C6	0.0314 (9)	0.0516 (10)	0.0464 (10)	−0.0002 (8)	0.0016 (8)	0.0028 (8)
C7A	0.0318 (9)	0.0366 (9)	0.0428 (9)	−0.0004 (7)	−0.0023 (7)	0.0006 (7)
C8	0.0473 (10)	0.0412 (9)	0.0441 (10)	−0.0039 (8)	−0.0090 (8)	0.0035 (8)

C9	0.0563 (12)	0.0558 (12)	0.0491 (12)	0.0041 (10)	−0.0073 (9)	−0.0021 (9)
C10	0.0704 (15)	0.0753 (15)	0.0464 (12)	−0.0061 (12)	−0.0033 (11)	−0.0041 (10)
C11	0.0880 (18)	0.0724 (15)	0.0483 (12)	−0.0084 (13)	−0.0192 (12)	0.0098 (11)
C12	0.0732 (16)	0.0726 (15)	0.0696 (16)	0.0122 (13)	−0.0266 (13)	0.0112 (12)
C13	0.0536 (12)	0.0649 (13)	0.0571 (13)	0.0087 (11)	−0.0106 (10)	0.0011 (10)

Geometric parameters (Å, º)

O1—C4	1.237 (2)	C3A—C4	1.426 (2)
N1—C7A	1.358 (2)	C6—H6	0.9300
N1—N2	1.376 (2)	C8—C9	1.377 (3)
N1—C8	1.428 (2)	C8—C13	1.384 (3)
N2—C3	1.321 (2)	C9—C10	1.377 (3)
N5—C6	1.355 (2)	C9—H9	0.9300
N5—C4	1.392 (2)	C10—C11	1.365 (4)
N5—H5	0.94 (3)	C10—H10	0.9300
N7—C6	1.304 (2)	C11—C12	1.376 (4)
N7—C7A	1.369 (2)	C11—H11	0.9300
C3—C3A	1.405 (2)	C12—C13	1.387 (3)
C3—H3	0.9300	C12—H12	0.9300
C3A—C7A	1.381 (2)	C13—H13	0.9300
C7A—N1—N2	110.66 (14)	N1—C7A—C3A	107.17 (15)
C7A—N1—C8	129.83 (16)	N7—C7A—C3A	127.16 (16)
N2—N1—C8	119.51 (15)	C9—C8—C13	120.60 (19)
C3—N2—N1	105.69 (14)	C9—C8—N1	119.61 (17)
C6—N5—C4	124.55 (16)	C13—C8—N1	119.79 (18)
C6—N5—H5	117.5 (15)	C8—C9—C10	119.4 (2)
C4—N5—H5	117.6 (15)	C8—C9—H9	120.3
C6—N7—C7A	111.62 (15)	C10—C9—H9	120.3
N2—C3—C3A	111.35 (17)	C11—C10—C9	120.9 (2)
N2—C3—H3	124.3	C11—C10—H10	119.5
C3A—C3—H3	124.3	C9—C10—H10	119.5
C7A—C3A—C3	105.13 (16)	C10—C11—C12	119.7 (2)
C7A—C3A—C4	119.32 (16)	C10—C11—H11	120.2
C3—C3A—C4	135.49 (18)	C12—C11—H11	120.2
O1—C4—N5	120.94 (16)	C11—C12—C13	120.6 (2)
O1—C4—C3A	127.74 (17)	C11—C12—H12	119.7
N5—C4—C3A	111.31 (16)	C13—C12—H12	119.7
N7—C6—N5	125.98 (17)	C8—C13—C12	118.8 (2)
N7—C6—H6	117.0	C8—C13—H13	120.6
N5—C6—H6	117.0	C12—C13—H13	120.6
N1—C7A—N7	125.67 (16)		
C7A—N1—N2—C3	−0.7 (2)	C6—N7—C7A—C3A	1.9 (3)
C8—N1—N2—C3	178.78 (16)	C3—C3A—C7A—N1	0.0 (2)
N1—N2—C3—C3A	0.7 (2)	C4—C3A—C7A—N1	177.64 (16)
N2—C3—C3A—C7A	−0.4 (2)	C3—C3A—C7A—N7	179.11 (18)

N2—C3—C3A—C4	−177.5 (2)	C4—C3A—C7A—N7	−3.2 (3)
C6—N5—C4—O1	178.24 (18)	C7A—N1—C8—C9	34.0 (3)
C6—N5—C4—C3A	−0.8 (3)	N2—N1—C8—C9	−145.37 (19)
C7A—C3A—C4—O1	−176.59 (18)	C7A—N1—C8—C13	−145.4 (2)
C3—C3A—C4—O1	0.2 (4)	N2—N1—C8—C13	35.2 (3)
C7A—C3A—C4—N5	2.3 (2)	C13—C8—C9—C10	1.0 (3)
C3—C3A—C4—N5	179.1 (2)	N1—C8—C9—C10	−178.44 (19)
C7A—N7—C6—N5	0.0 (3)	C8—C9—C10—C11	−0.7 (4)
C4—N5—C6—N7	−0.4 (3)	C9—C10—C11—C12	0.1 (4)
N2—N1—C7A—N7	−178.70 (17)	C10—C11—C12—C13	0.3 (4)
C8—N1—C7A—N7	1.9 (3)	C9—C8—C13—C12	−0.6 (3)
N2—N1—C7A—C3A	0.5 (2)	N1—C8—C13—C12	178.8 (2)
C8—N1—C7A—C3A	−178.97 (17)	C11—C12—C13—C8	0.0 (4)
C6—N7—C7A—N1	−179.11 (17)		

Hydrogen-bond geometry (Å, º)

*Cg*1 is the centroid of the C8–C13 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N5—H5···O1^{i}	0.94 (3)	1.94 (3)	2.862 (2)	166 (2)
C3—H3···O1^{ii}	0.93	2.28	3.180 (2)	162
C6—H6···N2^{iii}	0.93	2.48	3.374 (2)	162
C9—H9···*Cg*1^{iv}	0.93	2.94	3.767 (2)	150

Symmetry codes: (i) −*x*+2, −*y*+1, −*z*+1; (ii) −*x*+1, −*y*+1, −*z*+1; (iii) *x*+1, *y*, *z*; (iv) −*x*+3/2, *y*−1/2, *z*.