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Crystal structures and Hirshfeld surface analyses of 2-amino-4-(4-bromophenyl)-6-oxo-1-phenyl-1,4,5,6-tetrahydropyridine-3-carbonitrile hemihydrate and 1,6-diamino-2-oxo-4-phenyl-1,2-dihydropyridine-3,5-dicarbonitrile

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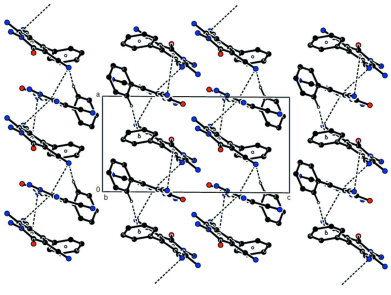
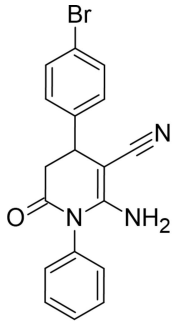
In 2-amino-4-(4-bromophenyl)-6-oxo-1-phenyl-1,4,5,6-tetrahydropyridine-3-carbonitrile hemihydrate, $C_{18}H_{14}BrN_3O{\cdot}0.5H_2O$, (I), pairs of molecules are linked by pairs of N—H···N hydrogen bonds, forming dimers with an $R_2^2(12)$ ring motif. The dimers are connected by N—H···Br and O—H···O hydrogen bonds, and C—Br···π interactions, forming layers parallel to the (010) plane. 1,6-Diamino-2-oxo-4-phenyl-1,2-dihydropyridine-3,5-dicarbonitrile, $C_{13}H_9N_5O$, (II), crystallizes in the triclinic space group $P\overline{1}$ with two independent molecules (IIA and IIB) in the asymmetric unit. In the crystal of (II), molecules IIA and IIB are linked by intermolecular N—H···N and N—H···O hydrogen bonds into layers parallel to (001). These layers are connected along the *c*-axis direction by weak C—H···N contacts. C—H···π and C—N···π interactions connect adjacent molecules, forming chains along the *a*-axis direction. In (I) and (II), the stability of the packing is ensured by van der Waals interactions between the layers. In (I), Hirshfeld surface analysis showed that the most important contributions to the crystal packing are from H···H (37.9%), C···H/H···C (18.4%), Br···H/H···Br (13.3%), N···H/H···N (11.5%) and O···H/H···O (10.0%) interactions, while in (II), H···H interactions are the most significant contributors to the crystal packing (27.6% for molecule IIA and 23.1% for molecule IIB).

1. Chemical context

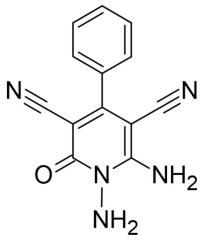
The formation of C—C, C—O, and C—N bonds is one of the essential transformation reactions of organic chemistry (Zubkov *et al.*, 2018; Shikhaliyev *et al.*, 2019; Viswanathan *et al.*, 2019; Gurbanov *et al.*, 2020). Nitrogen-containing heterocycles, especially tetrahydropyridine homologs, are well-known heterocyclic scaffolds that exhibit a broad spectrum of biological and pharmaceutical activities (Sośnicki & Idzik, 2019; Sangwan *et al.*, 2022). Being an important structural fragment of various natural products, they play a key role in cell metabolism. In view of the growing biological value of pyridine derivatives, we have considered the study of this class of compounds (Naghiyev *et al.*, 2020*b*) to be of great interest. Thus, in the framework of our ongoing structural studies



(Naghiyev *et al.*, 2020*a*,*b*, 2021, 2021*a*,*b*, 2022; Khalilov *et al.*, 2022), we report here the crystal structures and Hirshfeld surface analyses of 2-amino-4-(4-bromophenyl)-6-oxo-1-phenyl-1,4,5,6-tetrahydropyridine-3-carbonitrile hemihydrate (I) and 1,6-diamino-2-oxo-4-phenyl-1,2-dihydropyridine-3,5-dicarbonitrile (II).



(I)



(II)

2. Structural commentary

Compound (I) crystallizes in the monoclinic space group *C*2/*c* with $Z = 4$. In (I) (Fig. 1), the conformation of the central dihydropyridine ring is close to screw-boat with puckering parameters (Cremer & Pople, 1975) $Q_T = 0.4650\ (16)$ Å, $\theta = 61.3\ (2)^\circ$ and $\varphi = 211.4\ (2)^\circ$. The phenyl (C7–C12) and bromophenyl (C14–C19) rings form dihedral angles of 64.68 (8) and 88.25 (7)°, respectively, with the mean plane of the central dihydropyridine ring. The chirality about the C4 atom is *S* for this molecule, but both enantiomers are present in the crystal. The Br atom is disordered over two sites in a 0.59 (2):0.41 (2) ratio.

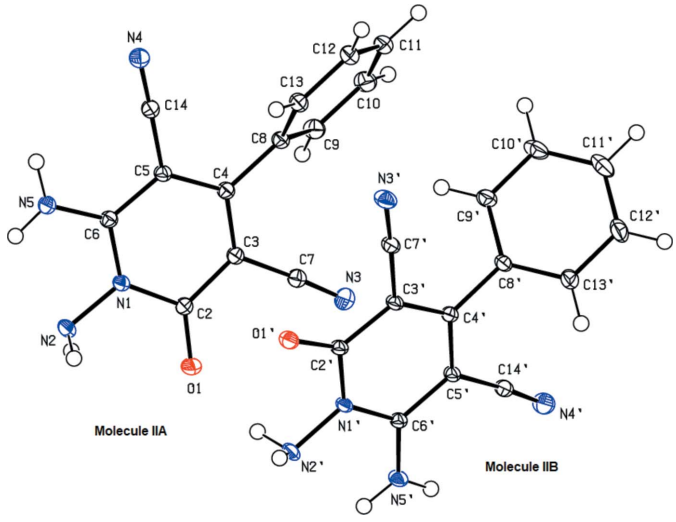


Figure 2
The molecular structure of compound (II). Displacement ellipsoids are drawn at the 50% probability level.

Compound (II) (Fig. 2) contains two independent molecules (IIA and IIB, atom labels for molecule IIB including the suffix ') in the asymmetric unit. Fig. 3 shows the overlay of molecules IIA and IIB (r.m.s. deviation = 0.210 Å). The pyridine and phenyl rings subtend dihedral angles of 52.95 (4)° in molecule IIA and 56.75 (3) ° in molecule IIB.

The geometric parameters of molecules (I), (IIA) and (IIB) are normal and comparable to those of related compounds listed in the *Database survey* section.

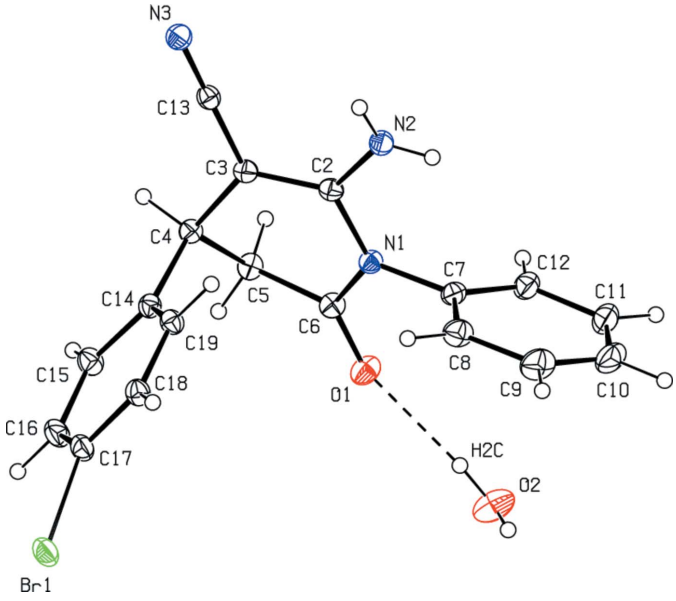


Figure 1
The molecular structure of compound (I) with displacement ellipsoids drawn at the 30% probability level. The O—H···O hydrogen bond is drawn with a dashed line. Only the major component of the bromide disorder is shown for clarity.

Figure 3
Overlay image of the two independent molecules (IIA and IIB) in the asymmetric unit of compound (II). Color code: carbon (gray), hydrogen (white), nitrogen (blue) and oxygen (red).

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···Br1^{i}	0.82 (2)	2.75 (2)	3.507 (3)	154.4 (19)
N2—H2A···Br1A^{i}	0.82 (2)	2.73 (2)	3.493 (4)	155.1 (19)
N2—H2B···N3^{ii}	0.84 (2)	2.24 (2)	3.0583 (18)	165 (2)
C5—H5B···N3^{iii}	0.99	2.59	3.5426 (19)	160
C8—H8···O2^{iv}	0.95	2.49	3.223 (2)	134
C12—H12···N3^{v}	0.95	2.65	3.411 (2)	138
C16—H16···N3^{vi}	0.95	2.62	3.5283 (19)	160
O2—H2C···O1	0.85 (1)	2.09 (2)	2.8739 (14)	153 (3)

Symmetry codes: (i) $x, -y+2, z+\frac{1}{2}$; (ii) $-x+\frac{3}{2}, -y+\frac{5}{2}, -z+1$; (iii) $x, y-1, z$; (iv) $x, y+1, z$; (v) $-x+\frac{3}{2}, -y+\frac{3}{2}, -z+1$; (vi) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$.

3. Supramolecular features

In (I), pairs of N—H···N hydrogen bonds connect the molecules, forming dimers with an $R_2^2(12)$ ring motif (Fig. 4, Table 1). Further N—H···Br and O—H···O hydrogen bonds, as well as C—Br···π interactions [C17—Br1···$Cg2^{vii}$: Br1···$Cg2^{vii}$ = 3.493 (2) Å, C17···$Cg2^{vii}$ = 5.3027 (18) Å, C17—Br1···$Cg2^{vii}$ = 157.80 (14)°; C17—Br1A···$Cg2^{vii}$: Br1A···$Cg2^{vii}$ = 3.434 (6) Å, C17···$Cg2^{vii}$ = 5.3027 (18) Å, C17—Br1A···$Cg2^{vii}$ = 164.8 (3)°; symmetry code: (vii) $x, 2-y, -z+\frac{1}{2}$; $Cg2$ is the centroid of the C7–C12 phenyl ring], link the dimers, forming layers parallel to the (010) plane (Fig. 4). Interlayer van der Waals interactions strengthen the molecular packing.

In the crystal of (II), molecules IIA and IIB are linked by intermolecular N—H···N and N—H···O hydrogen bonds

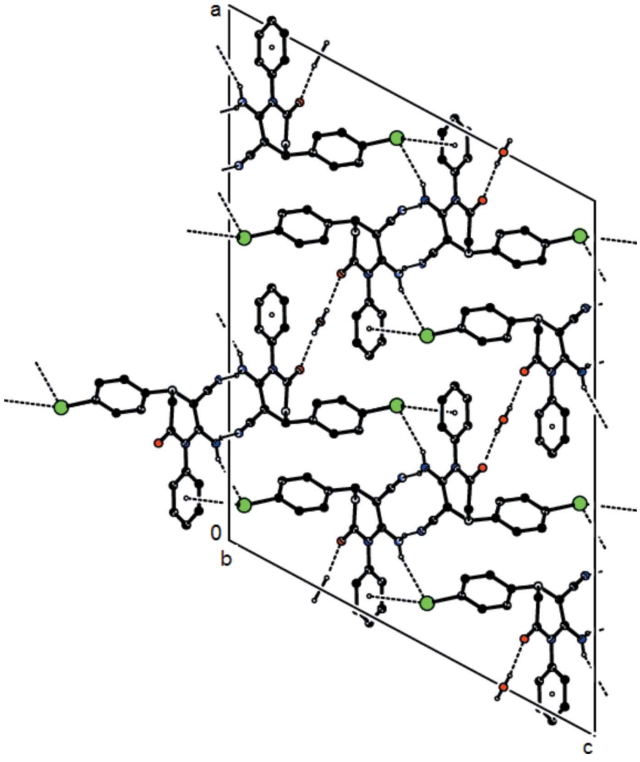


Figure 4
Crystal packing of compound (I) viewed down the b axis, showing the O—H···O, N—H···O and C—Br···π interactions.

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

$Cg2$ is the centroid of the C8–C13 phenyl ring.

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···N4^{i}	0.913 (13)	2.541 (13)	3.3713 (9)	151.6 (11)
N2—H2B···N4^{ii}	0.916 (14)	2.495 (14)	3.2404 (10)	138.7 (11)
N2—H2B···O1^{iii}	0.916 (14)	2.381 (13)	3.0650 (8)	131.5 (11)
N5—H5A···N3′^{ii}	0.897 (14)	2.525 (14)	3.1431 (9)	126.6 (11)
N5—H5B···O1′^{ii}	0.930 (14)	1.986 (14)	2.8853 (8)	162.3 (12)
N2′—H2A′···O1′^{iv}	0.898 (13)	2.186 (13)	3.0608 (8)	164.4 (11)
N2′—H2B′···N2^{iii}	0.902 (15)	2.681 (14)	3.1829 (8)	116.1 (10)
N2′—H2B′···O1	0.902 (15)	2.250 (15)	3.1373 (9)	167.5 (12)
N5′—H5A′···N3′^{i}	0.887 (15)	2.102 (15)	2.9314 (8)	155.2 (13)
C9′—H9′···$Cg2$	0.95	2.93	3.7972 (5)	153

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

(Table 2) into layers parallel to (001). These layers are connected along the c-axis direction by weak C—H···N contacts. Furthermore, C—H···π (Table 1) and C—N···π [C7—N3···$Cg3$: N3···$Cg3$ = 3.0831 (8) Å, C7···$Cg3$ = 3.3390 (8) Å, C7—N3···$Cg3$ = 92.50 (5)°; C7′—N3′···$Cg1^{v}$: N3′···$Cg1^{v}$ = 3.4626 (9) Å, C7′···$Cg1^{v}$ = 3.7591 (9) Å, C7′—N3′···$Cg1^{v}$ = 95.78 (6)°; C14—N4···$Cg3^{vi}$: N4···$Cg3^{vi}$ = 3.3807 (7) Å, C14···$Cg3^{vi}$ = 3.8513 (7) Å, C14—N4···$Cg3^{vi}$ = 105.23 (5)°; symmetry codes: (v) $1+x, y, z$, (vi) $-1+x, 1+y, z$; where $Cg1$ and $Cg3$ are the centroids of the N1/C2 –C6 and N1′/C2′ –C6′ pyridine rings of molecules IIA and IIB, respectively] interactions connect the adjacent molecules, forming chains along the a-axis direction (Fig. 5). The stability of the molecular packaging is ensured by van der Waals interactions between the layers.

4. Hirshfeld surface analyses

CrystalExplorer17.5 (Turner *et al.*, 2017) was used to construct Hirshfeld surfaces and generate the related two-dimensional fingerprint plots to illustrate the intermolecular interactions

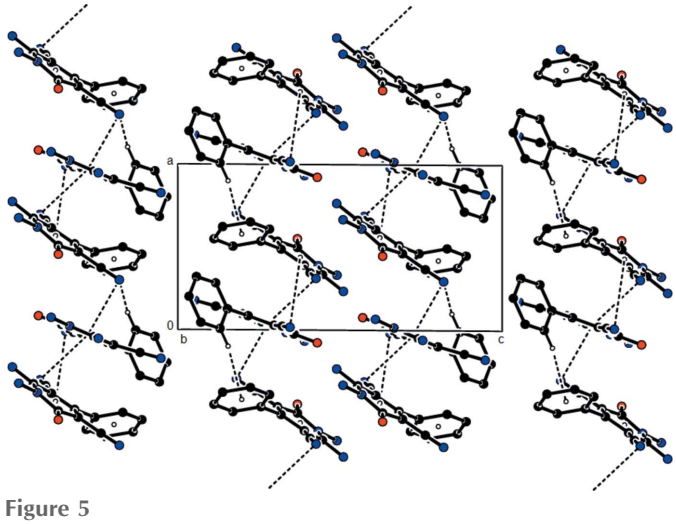


Figure 5
View down the b axis of compound (II) showing the C—H···π and C—N···π hydrogen bonds (dashed lines). The intramolecular C—N···π interaction in molecule IIA is omitted for clarity.

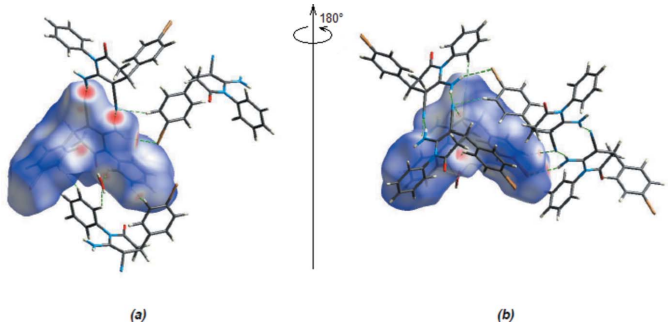


Figure 6
(*a*) Front and (*b*) back views of the Hirshfeld surfaces mapped over d_{norm} for (I).

for molecules (I) and (II). The d_{norm} mappings of (I) were conducted in the range −0.4915 to +1.2143 a.u. Bright-red circles on the d_{norm} surfaces (Fig. 6*a*,*b*) represent N—H···O and O—H···O interaction zones. Red areas on the Hirshfeld surfaces are also caused by the N—H···Br and C—H···N interactions (Tables 1 and 3).

Table 3
Summary of short interatomic contacts (Å) in compound (I).

Contact	Distance	Symmetry operation
Br1*A*···H2*A*	2.73	$x, 2-y, -\frac{1}{2}+z$
O1···H2*C*	2.09	$1-x, y, \frac{1}{2}-z$
O1···H19	2.40	$x, -1+y, z$
N3···H2*B*	2.24	$\frac{3}{2}-x, \frac{5}{2}-y, 1-z$
H12···N3	2.65	$\frac{3}{2}-x, \frac{5}{2}-y, 1-z$
N3···H16	2.62	$\frac{3}{2}-x, \frac{1}{2}+y, \frac{1}{2}-z$
H8···O2	2.49	$x, 1+y, z$
H9···C18	2.69	$1-x, y, \frac{1}{2}-z$
O2···O1	2.87	$1-x, y, \frac{1}{2}-z$

The fingerprint plots of (I) (Fig. 7) show that, while H···H (37.9%; Fig. 7*b*) interactions provide the highest contribution (Table 3), as would be expected for a molecule with so many H atoms, C···H/H···C (18.4%; Fig. 7*c*), Br···H/H···Br (13.3%; Fig. 7*d*), N···H/H···N (11.5%; Fig. 7*e*) and O···H/H···O (10.0%; Fig. 7*f*) contacts are also significant. Table 5 shows the contributions of all contacts.

In (II), the d_{norm} mappings for molecules IIA and IIB were performed in the ranges −0.5399 to 1.2085 a.u. and −0.5388 to 1.1921 a.u., respectively. The locations of N—H···N interactions are shown by bright red circles on the d_{norm} surfaces (Fig. 8*a*,*b* for A and Fig. 8*c*,*d* for B). Red spots on the

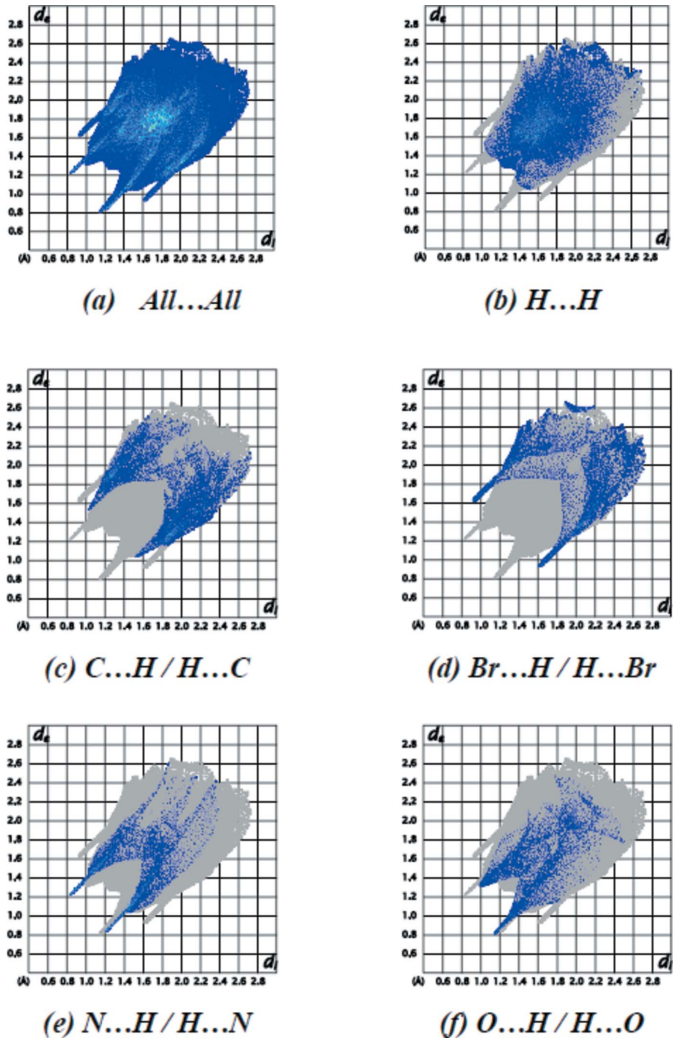


Figure 7
The two-dimensional fingerprint plots of (I), showing all interactions (*a*), and those delineated into H···H (*b*), C···H/H···C (*c*), Br···H/H···Br (*d*), N···H/H···N (*e*) and O···H/H···O (*f*) interactions. The d_i and d_e values are the closest internal and external distances (in Å) from given points on the Hirshfeld surfaces.

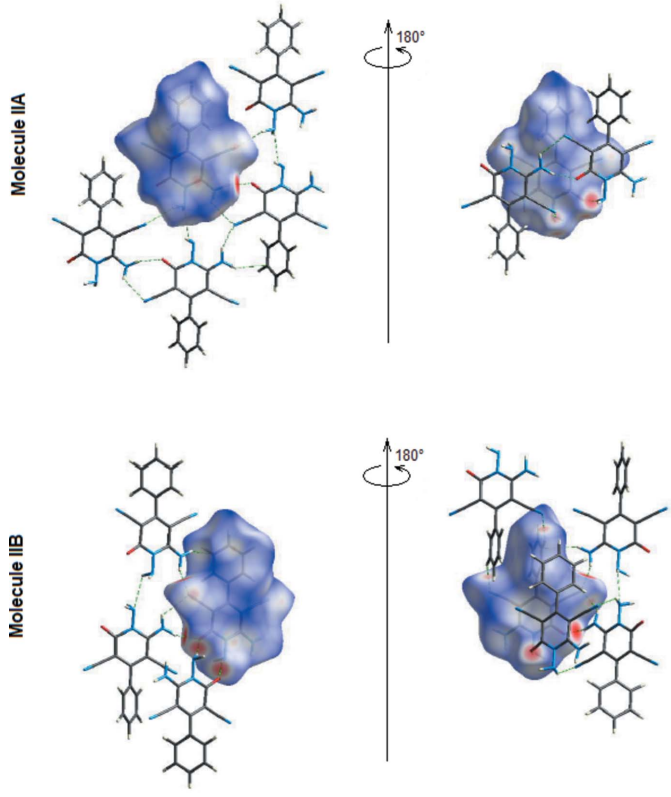


Figure 8
Front and back views of the three-dimensional Hirshfeld surface of molecules (IIA) and (IIB) plotted over d_{norm} in the range −0.5399 to 1.2085 a.u. for (IIA) and in the range −0.5388 to 1.1921 a.u. for (IIB).

Table 4
Summary of short interatomic contacts (Å) in compound (II).

Contact	Distance	Symmetry operation
O1···H2*B*′	2.25	*x*, *y*, *z*
H2*A*···N4	2.54	*x*, −1 + *y*, *z*
H2*B*···O1	2.38	1 − *x*, −*y*, 1 − *z*
H13···H5*A*	2.46	1 − *x*, 1 − *y*, 1 − *z*
N2···H2*B*′	2.68	1 − *x*, −*y*, 1 − *z*
H10···H12′	2.46	2 − *x*, 1 − *y*, −*z*
N4···H2*A*′	2.82	−1 + *x*, 1 + *y*, *z*
H5*B*···O1′	1.99	1 − *x*, 1 − *y*, 1 − *z*
H9···C12′	2.83	−1 + *x*, *y*, *z*
H12···N5′	2.89	*x*, 1 + *y*, *z*
H2*A*′···O1′	2.19	2 − *x*, −*y*, 1 − *z*
N3′···H5*A*′	2.10	1 + *x*, *y*, *z*
H10′···N4′	2.55	2 − *x*, 1 − *y*, −*z*
H12′···H12′	2.36	3 − *x*, 1 − *y*, −*z*

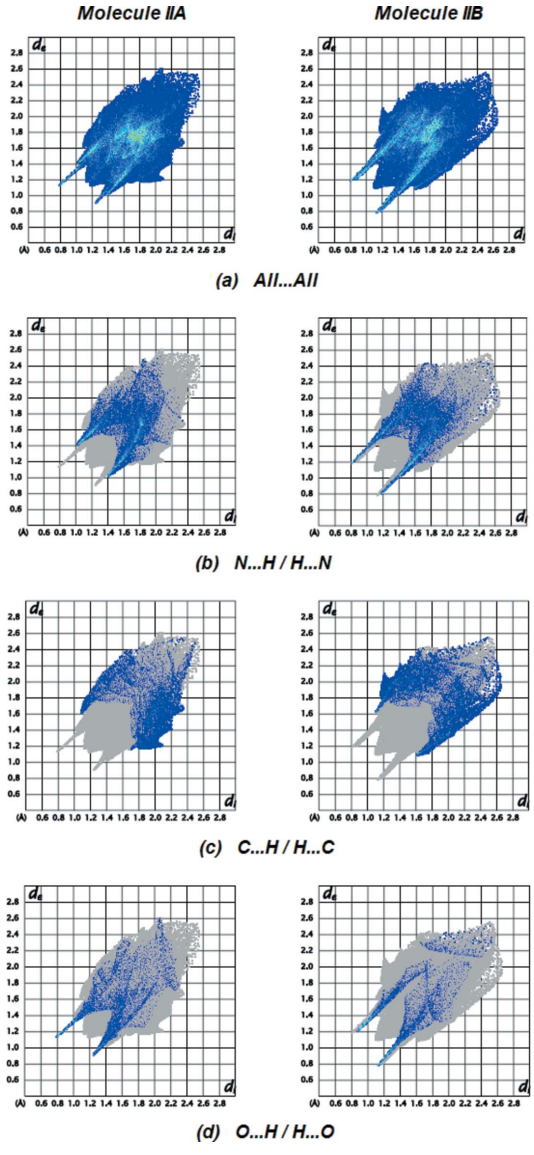


Figure 9
The full two-dimensional fingerprint plots for molecules (IIA) and (IIB), showing all interactions (*a*) and those delineated into N···H/H···N (*b*), C···H/H···C (*c*) and O···H/H···O (*d*) interactions. The d_i and d_e values are the closest internal and external distances (in Å) from given points on the Hirshfeld surface.

Table 5
Percentage contributions of interatomic contacts to the Hirshfeld surface for compound (I).

Contact	Percentage contribution
H···H	37.9
C···H/H···C	18.4
Br···H/H···Br	13.3
N···H/H···N	11.5
O···H/H···O	10.0
Br···C/C···Br	4.2
C···C	1.5
N···C/C···N	1.3
N···N	0.8
Br···Br	0.6
C···O/O···C	0.5

Table 6
Percentage contributions of interatomic contacts to the Hirshfeld surface for compound (II).

Contact	% contribution for IIA	% contribution for IIB
H···H	27.6	23.1
N···H/H···N	25.2	28.3
C···H/H···C	15.2	21.2
O···H/H···O	11.4	8.8
N···C/C···N	8.6	6.7
C···C	6.8	7.5
N···N	2.1	2.8
N···O/O···N	1.7	0.6
C···O/O···C	1.3	0.9

Hirshfeld surfaces are also caused by N—H···O interactions (Tables 2 and 4).

Fig. 9 displays the full two-dimensional fingerprint plot and those delineated into the major contacts. H···H interactions (Fig. 9*b*; 27.6% contribution for IIA; 23.1% for IIB) are the major factor in the crystal packing with N···H/H···N (Fig. 9*c*; 25.2% for IIA; 28.3% for IIB), C···H/H···C (Fig. 9*d*; 15.2% for IIA; 21.2% for IIB) and O···H/H···O (Fig. 9*e*; 11.4% for IIA; 8.8% for IIB) interactions representing the next highest contributions. The percentage contributions of comparative weaker interactions of molecules IIA and IIB are given in Table 6. The surroundings of molecules IIA and IIB are quite similar, as seen by the data comparison.

5. Database survey

A search of the Cambridge Structural Database (CSD, Version 5.42, update of September 2021; Groom *et al.*, 2016) gave eleven compounds closely related to the title compounds, *viz.* CSD refcodes YAXQAT (**I**) (Mamedov *et al.*, 2022), OZAKOS (**II**) (Naghiyev *et al.*, 2021), JEBREQ (**III**) (Mohana *et al.*, 2017), JEBRAM (**IV**) (Mohana *et al.*, 2017), SETWUK (**V**) (Suresh *et al.*, 2007), SETWOE (**VI**) (Suresh *et al.*, 2007), IQEFOC (**VII**) (Naghiyev *et al.*, 2021*a*), MOKBUL (**VIII**) (Mohamed *et al.*, 2014), PAVQIO (**IX**) (Al-Said *et al.*, 2012), YIZGOE01 (**X**) (Jia & Tu, 2008) and YIBZAL (**XI**) (Eyduran *et al.*, 2007).

In the crystal of (**I**) (space group: *Pc*), the two molecules in the asymmetric unit are joined together by N—H···O hydrogen bonds, forming a dimer with an $R_2^2(16)$ ring motif.

Table 7
Experimental details.

	(I)	(II)
Crystal data		
Chemical formula	$2C_{18}H_{14}BrN_3O{\cdot}H_2O$	$C_{13}H_9N_5O$
M_r	754.48	251.25
Crystal system, space group	Monoclinic, *C*2/*c*	Triclinic, $P\overline{1}$
Temperature (K)	100	100
a, *b*, *c* (Å)	27.539 (3), 6.3430 (6), 21.3540 (19)	8.6444 (1), 8.9104 (2), 16.0902 (2)
α, β, γ (°)	90, 118.170 (12), 90	79.196 (1), 86.485 (1), 69.003 (2)
V (Å^3)	3288.2 (6)	1136.52 (4)
Z	4	4
Radiation type	Synchrotron, λ = 0.74500 Å	Mo *K*α
μ (mm^{-1})	2.83	0.10
Crystal size (mm)	0.10 × 0.07 × 0.05	0.15 × 0.12 × 0.06
Data collection		
Diffractometer	Rayonix SX-165 CCD	XtaLAB Synergy, Dualflex, HyPix
Absorption correction	Multi-scan (*SCALA*; Evans, 2006)	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2021)
T_{min}, T_{max}	0.742, 0.851	0.972, 0.980
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	28485, 4492, 4047	88754, 9666, 8561
R_{int}	0.025	0.029
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.692	0.816
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.031, 0.086, 1.06	0.039, 0.118, 1.03
No. of reflections	4492	9666
No. of parameters	233	363
No. of restraints	2	0
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.45, −0.43	0.54, −0.31

Computer programs: *Marccd* (Doyle, 2011), *CrysAlis PRO* (Rigaku OD, 2021), *iMosflm* (Battye *et al.*, 2011), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*), *ORTEP-3 for Windows* (Farrugia, 2012), and *PLATON* (Spek, 2020).

N—H···O and N—H···N hydrogen bonds link the dimers, generating chains along the *c*-axis direction, which are connected by C—Br···π interactions. In (**II**) (space group: *Pc*), intermolecular N—H···N and C—H···N hydrogen bonds, as well as N—H···π and C—H···π interactions, connect molecules in the crystal, generating a 3D network. In both (**III**) (space group: $P\overline{1}$) and (**IV**) (space group: $P\overline{1}$), a supramolecular homosynthon [$R_2^2(8)$ ring motif] is formed through N—H···N hydrogen bonds. The molecular structures are further stabilized by π–π stacking, and C=O···π, C—H···O and C—H···Cl interactions. In (**V**) (space group: $P2_1/n$), the crystal structure is stabilized by intermolecular C—H···F and C—H···π interactions, and in (**VI**) (space group: $P2_1/c$), by intermolecular C—H···O and C—H···π interactions. In (**VII**) (space group: *Cc*), intermolecular N—H···N and C—H···N hydrogen bonds form molecular sheets parallel to the (110) and (110) planes, crossing each other. Adjacent molecules are further linked by C—H···π interactions, which form zigzag chains propagating parallel to [100]. The compound (**VIII**) (space group: $Pca2_1$) crystallizes with two independent molecules, *A* and *B*, in the asymmetric unit. In the crystal, molecules *A* and *B* are linked by N—H···S, N—H···N and C—H···S hydrogen bonds, forming a three-dimensional network. In (**IX**) (space group: $P2_1/c$), molecules are linked into a chain along the *b*-axis direction *via* C—H···O interactions. In (**X**) (space group: $P\overline{1}$), the crystal packing is stabilized by intermolecular N—H···N, O—H···O and N—H···O hydrogen bonds. In (**XI**) (space group: $P2_1/c$), the molecules form centrosymmetric dimers *via* N—H···S hydrogen bonds.

6. Synthesis and crystallization

Compounds (I) and (II) were synthesized using reported procedures [Mamedov *et al.* (2020) and Soto *et al.* (1981), respectively]. Colorless crystals of (I) were obtained at room temperature upon slow evaporation of a homogeneous methanol solution, while colorless needle-like crystals of (II) were obtained at room temperature upon slow evaporation from an ethanol/water (3:1) homogeneous solution.

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 7. In (I), the H atoms were placed at calculated positions (C—H = 0.95–1.00 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(C-methyl). The N-bound H atoms and the H atoms of the water molecule located at the coordinates (0.5, *y*, 0.25) were found in a difference-Fourier map, and refined freely [N2—H2*A* = 0.82 (2), N2—H2*B* = 0.84 (2) Å, and O2—H2*C* = 0.849 (10), O2—H2*C*($-x+1$, *y*, $-z+\frac{1}{2}$) = 0.849 (10) Å, with U_{iso}(H) = 1.2 or 1.5U_{eq}(N, O). The DFIX instruction was applied to constrain

the distance O2—H2*C*. The Br1 atom is disordered over two positions with refined occupancies of 0.59 (2) and 0.41 (2).

In (II), the H atoms were placed at calculated positions (C—H = 0.95 Å) and refined using a riding model with U_{iso}(H) = 1.2U_{eq}(C). N-bound H atoms were found in a difference Fourier map and refined freely [N2—H2*A* = 0.913 (13), N2—H2*B* = 0.916 (14), N5—H5*A* = 0.897 (14) and N5—H5*B* = 0.930 (14) Å for molecule IIA, and N2′—H2*A*′ = 0.898 (13), N2′—H2*B*′ = 0.902 (15), N5′—H5*A*′ = 0.887 (15) and N5′—H5*B*′ = 0.889 (12) Å for molecule IIB].

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supporting information

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Crystal structures and Hirshfeld surface analyses of 2-amino-4-(4-bromophenyl)-6-oxo-1-phenyl-1,4,5,6-tetrahydropyridine-3-carbonitrile hemihydrate and 1,6-diamino-2-oxo-4-phenyl-1,2-dihydropyridine-3,5-dicarbonitrile

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Computing details

Data collection: *Marccd* (Doyle, 2011) for (I); *CrysAlis PRO* (Rigaku OD, 2021) for (II). Cell refinement: *iMosflm* (Battye *et al.*, 2011) for (I); *CrysAlis PRO* (Rigaku OD, 2021) for (II). Data reduction: *iMosflm* (Battye *et al.*, 2011) for (I); *CrysAlis PRO* (Rigaku OD, 2021) for (II). For both structures, program(s) used to solve structure: SHELXT (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL* (Sheldrick, 2015b); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *PLATON* (Spek, 2020).

2-Amino-4-(4-bromophenyl)-6-oxo-1-phenyl-1,4,5,6-tetrahydropyridine-3-carbonitrile hemihydrate (I)

Crystal data

$2C_{18}H_{14}BrN_3O·H_2O$
M_r = 754.48
Monoclinic, $C2/c$
a = 27.539 (3) Å
b = 6.3430 (6) Å
c = 21.3540 (19) Å
β = 118.170 (12)°
V = 3288.2 (6) Å^3
Z = 4
$F(000)$ = 1528
D_x = 1.524 Mg m^{-3}
Synchrotron radiation, λ = 0.74500 Å
Cell parameters from 1000 reflections
θ = 1.8–24.0°
μ = 2.83 mm^{-1}
T = 100 K
Prism, yellow
0.10 × 0.07 × 0.05 mm

Data collection

Rayonix SX-165 CCD diffractometer
/f scan
Absorption correction: multi-scan (*SCALA*; Evans, 2006)
T_{min} = 0.742, T_{max} = 0.851
28485 measured reflections
4492 independent reflections
4047 reflections with $I > 2\sigma(I)$
R_{int} = 0.025
θ_{max} = 31.0°, θ_{min} = 1.8°
h = −38→38
k = −8→8
l = −29→29

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.086
S = 1.06
4492 reflections
233 parameters
2 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0485P)^2 + 2.5862P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.45$ e Å^{-3}
$\Delta\rho_{min} = -0.43$ e Å^{-3}

Extinction correction: SHELXL-2018/3 (Sheldrick, 2015b), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0066 (5)

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Br1	0.58033 (10)	1.0754 (4)	0.04138 (12)	0.0362 (3)	0.59 (2)
Br1A	0.5838 (2)	1.1121 (17)	0.0450 (2)	0.0521 (7)	0.41 (2)
O1	0.61090 (5)	0.37633 (17)	0.30715 (7)	0.0337 (3)	
N1	0.63725 (5)	0.65818 (18)	0.38065 (6)	0.0224 (2)	
N2	0.66784 (6)	0.9297 (2)	0.46401 (7)	0.0259 (2)	
H2A	0.6410 (10)	0.904 (3)	0.4699 (12)	0.031*	
H2B	0.6843 (9)	1.044 (3)	0.4797 (11)	0.031*	
N3	0.78997 (5)	1.13330 (19)	0.47344 (7)	0.0273 (2)	
C2	0.67632 (6)	0.8155 (2)	0.41704 (7)	0.0221 (2)	
C3	0.71957 (6)	0.8467 (2)	0.40309 (7)	0.0228 (2)	
C4	0.72370 (6)	0.7256 (2)	0.34490 (7)	0.0222 (2)	
H4	0.763385	0.716345	0.356821	0.027*	
C5	0.70242 (6)	0.5023 (2)	0.34527 (8)	0.0248 (3)	
H5A	0.700533	0.422449	0.304338	0.030*	
H5B	0.728708	0.428933	0.389238	0.030*	
C6	0.64645 (6)	0.5040 (2)	0.34127 (8)	0.0248 (3)	
C7	0.58549 (6)	0.6519 (2)	0.38258 (7)	0.0249 (3)	
C8	0.54681 (7)	0.8076 (3)	0.34787 (9)	0.0339 (3)	
H8	0.554201	0.918309	0.323626	0.041*	
C9	0.49690 (8)	0.7984 (3)	0.34924 (11)	0.0446 (4)	
H9	0.470156	0.905529	0.326486	0.053*	
C10	0.48580 (7)	0.6351 (3)	0.38334 (11)	0.0442 (4)	
H10	0.451308	0.629490	0.383299	0.053*	
C11	0.52464 (7)	0.4800 (3)	0.41753 (10)	0.0382 (4)	
H11	0.516806	0.367789	0.440849	0.046*	
C12	0.57518 (7)	0.4881 (2)	0.41780 (9)	0.0304 (3)	
H12	0.602285	0.382964	0.441729	0.037*	
C13	0.75857 (6)	1.0032 (2)	0.44177 (7)	0.0230 (2)	
C14	0.69159 (6)	0.8247 (2)	0.27130 (7)	0.0222 (2)	
C15	0.69605 (6)	0.7419 (2)	0.21353 (8)	0.0284 (3)	
H15	0.721123	0.629945	0.220994	0.034*	
C16	0.66441 (7)	0.8207 (3)	0.14545 (8)	0.0320 (3)	
H16	0.667074	0.761790	0.106281	0.038*	
C17	0.62892 (6)	0.9867 (3)	0.13569 (8)	0.0293 (3)	

C18	0.62500 (6)	1.0777 (2)	0.19181 (8)	0.0264 (3)
H18	0.601436	1.194973	0.184383	0.032*
C19	0.65621 (6)	0.9943 (2)	0.25941 (7)	0.0235 (3)
H19	0.653345	1.054266	0.298300	0.028*
O2	0.500000	0.2217 (3)	0.250000	0.0497 (5)
H2C	0.5274 (8)	0.305 (4)	0.2670 (16)	0.075*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0326 (4)	0.0536 (6)	0.0240 (3)	0.0061 (6)	0.0149 (3)	0.0099 (3)
Br1A	0.0486 (12)	0.0873 (19)	0.0298 (7)	0.0336 (9)	0.0262 (7)	0.0238 (8)
O1	0.0301 (6)	0.0284 (5)	0.0446 (6)	−0.0049 (4)	0.0193 (5)	−0.0142 (4)
N1	0.0219 (5)	0.0217 (5)	0.0239 (5)	−0.0008 (4)	0.0109 (4)	−0.0025 (4)
N2	0.0274 (6)	0.0263 (5)	0.0266 (6)	−0.0044 (5)	0.0149 (5)	−0.0058 (4)
N3	0.0290 (6)	0.0255 (5)	0.0276 (6)	−0.0020 (5)	0.0133 (5)	−0.0005 (4)
C2	0.0238 (6)	0.0203 (5)	0.0205 (5)	0.0009 (4)	0.0090 (5)	0.0005 (4)
C3	0.0235 (6)	0.0221 (5)	0.0216 (6)	−0.0002 (5)	0.0096 (5)	−0.0003 (4)
C4	0.0220 (6)	0.0212 (5)	0.0239 (6)	0.0014 (4)	0.0112 (5)	−0.0004 (4)
C5	0.0259 (7)	0.0200 (5)	0.0298 (6)	0.0031 (5)	0.0142 (5)	0.0004 (5)
C6	0.0259 (7)	0.0204 (5)	0.0278 (6)	0.0009 (5)	0.0126 (5)	−0.0015 (5)
C7	0.0208 (6)	0.0277 (6)	0.0254 (6)	−0.0014 (5)	0.0102 (5)	−0.0055 (5)
C8	0.0285 (8)	0.0374 (8)	0.0329 (7)	0.0058 (6)	0.0122 (6)	−0.0010 (6)
C9	0.0278 (8)	0.0549 (10)	0.0469 (10)	0.0111 (7)	0.0143 (7)	−0.0055 (8)
C10	0.0258 (8)	0.0594 (11)	0.0507 (10)	−0.0063 (7)	0.0207 (8)	−0.0189 (9)
C11	0.0336 (8)	0.0426 (9)	0.0448 (9)	−0.0120 (7)	0.0238 (7)	−0.0119 (7)
C12	0.0277 (7)	0.0303 (7)	0.0350 (7)	−0.0053 (6)	0.0162 (6)	−0.0049 (6)
C13	0.0247 (6)	0.0229 (6)	0.0221 (6)	0.0020 (5)	0.0116 (5)	0.0021 (5)
C14	0.0230 (6)	0.0213 (5)	0.0241 (6)	−0.0007 (5)	0.0125 (5)	−0.0010 (4)
C15	0.0299 (7)	0.0300 (6)	0.0290 (7)	0.0052 (5)	0.0169 (6)	−0.0007 (5)
C16	0.0325 (8)	0.0429 (8)	0.0259 (7)	0.0041 (6)	0.0182 (6)	−0.0009 (6)
C17	0.0271 (7)	0.0396 (7)	0.0227 (6)	0.0028 (6)	0.0132 (5)	0.0068 (6)
C18	0.0275 (7)	0.0263 (6)	0.0268 (6)	0.0026 (5)	0.0139 (6)	0.0036 (5)
C19	0.0274 (7)	0.0218 (6)	0.0232 (6)	0.0002 (5)	0.0135 (5)	−0.0009 (5)
O2	0.0349 (10)	0.0329 (9)	0.0631 (13)	0.000	0.0082 (9)	0.000

Geometric parameters (Å, º)

Br1—C17	1.902 (3)	C8—C9	1.390 (2)
Br1A—C17	1.912 (4)	C8—H8	0.9500
O1—C6	1.2131 (18)	C9—C10	1.381 (3)
N1—C6	1.3886 (17)	C9—H9	0.9500
N1—C2	1.4027 (17)	C10—C11	1.381 (3)
N1—C7	1.4460 (18)	C10—H10	0.9500
N2—C2	1.3440 (17)	C11—C12	1.390 (2)
N2—H2A	0.82 (2)	C11—H11	0.9500
N2—H2B	0.84 (2)	C12—H12	0.9500
N3—C13	1.1551 (19)	C14—C19	1.3921 (18)

C2—C3	1.3716 (19)	C14—C15	1.3986 (18)
C3—C13	1.4080 (19)	C15—C16	1.388 (2)
C3—C4	1.5101 (18)	C15—H15	0.9500
C4—C14	1.5278 (19)	C16—C17	1.384 (2)
C4—C5	1.5347 (18)	C16—H16	0.9500
C4—H4	1.0000	C17—C18	1.380 (2)
C5—C6	1.5031 (19)	C18—C19	1.390 (2)
C5—H5A	0.9900	C18—H18	0.9500
C5—H5B	0.9900	C19—H19	0.9500
C7—C8	1.383 (2)	O2—H2C	0.849 (10)
C7—C12	1.389 (2)	O2—H2C^{i}	0.849 (10)

C6—N1—C2	121.67 (12)	C10—C9—H9	119.7
C6—N1—C7	117.52 (11)	C8—C9—H9	119.7
C2—N1—C7	120.82 (11)	C9—C10—C11	120.26 (16)
C2—N2—H2A	119.6 (14)	C9—C10—H10	119.9
C2—N2—H2B	120.8 (15)	C11—C10—H10	119.9
H2A—N2—H2B	118 (2)	C10—C11—C12	120.00 (17)
N2—C2—C3	123.97 (13)	C10—C11—H11	120.0
N2—C2—N1	116.02 (12)	C12—C11—H11	120.0
C3—C2—N1	120.00 (12)	C7—C12—C11	119.05 (16)
C2—C3—C13	118.33 (12)	C7—C12—H12	120.5
C2—C3—C4	121.03 (12)	C11—C12—H12	120.5
C13—C3—C4	120.55 (12)	N3—C13—C3	179.02 (15)
C3—C4—C14	113.92 (11)	C19—C14—C15	118.33 (13)
C3—C4—C5	106.75 (11)	C19—C14—C4	121.39 (11)
C14—C4—C5	110.35 (11)	C15—C14—C4	120.26 (12)
C3—C4—H4	108.6	C16—C15—C14	121.04 (13)
C14—C4—H4	108.6	C16—C15—H15	119.5
C5—C4—H4	108.6	C14—C15—H15	119.5
C6—C5—C4	112.13 (11)	C17—C16—C15	118.77 (13)
C6—C5—H5A	109.2	C17—C16—H16	120.6
C4—C5—H5A	109.2	C15—C16—H16	120.6
C6—C5—H5B	109.2	C18—C17—C16	121.80 (13)
C4—C5—H5B	109.2	C18—C17—Br1	119.43 (14)
H5A—C5—H5B	107.9	C16—C17—Br1	118.58 (14)
O1—C6—N1	120.51 (13)	C18—C17—Br1A	115.2 (2)
O1—C6—C5	122.98 (12)	C16—C17—Br1A	123.0 (2)
N1—C6—C5	116.49 (12)	C17—C18—C19	118.64 (13)
C8—C7—C12	121.46 (14)	C17—C18—H18	120.7
C8—C7—N1	119.04 (13)	C19—C18—H18	120.7
C12—C7—N1	119.49 (13)	C18—C19—C14	121.34 (12)
C7—C8—C9	118.56 (17)	C18—C19—H19	119.3
C7—C8—H8	120.7	C14—C19—H19	119.3
C9—C8—H8	120.7	H2C—O2—H2C^{i}	103 (4)
C10—C9—C8	120.66 (17)		

C6—N1—C2—N2	−167.48 (13)	C12—C7—C8—C9	0.5 (2)

C7—N1—C2—N2	12.90 (18)	N1—C7—C8—C9	179.12 (14)
C6—N1—C2—C3	13.26 (19)	C7—C8—C9—C10	−1.3 (3)
C7—N1—C2—C3	−166.35 (13)	C8—C9—C10—C11	0.9 (3)
N2—C2—C3—C13	2.1 (2)	C9—C10—C11—C12	0.1 (3)
N1—C2—C3—C13	−178.68 (12)	C8—C7—C12—C11	0.5 (2)
N2—C2—C3—C4	−174.42 (13)	N1—C7—C12—C11	−178.07 (13)
N1—C2—C3—C4	4.77 (19)	C10—C11—C12—C7	−0.8 (2)
C2—C3—C4—C14	85.13 (15)	C3—C4—C14—C19	−8.24 (18)
C13—C3—C4—C14	−91.35 (15)	C5—C4—C14—C19	111.81 (14)
C2—C3—C4—C5	−36.93 (16)	C3—C4—C14—C15	173.58 (13)
C13—C3—C4—C5	146.59 (12)	C5—C4—C14—C15	−66.37 (16)
C3—C4—C5—C6	52.57 (15)	C19—C14—C15—C16	−2.6 (2)
C14—C4—C5—C6	−71.70 (14)	C4—C14—C15—C16	175.64 (14)
C2—N1—C6—O1	−176.04 (13)	C14—C15—C16—C17	1.3 (2)
C7—N1—C6—O1	3.6 (2)	C15—C16—C17—C18	1.2 (2)
C2—N1—C6—C5	5.58 (18)	C15—C16—C17—Br1	−173.74 (14)
C7—N1—C6—C5	−174.79 (12)	C15—C16—C17—Br1A	179.2 (4)
C4—C5—C6—O1	141.73 (14)	C16—C17—C18—C19	−2.4 (2)
C4—C5—C6—N1	−39.93 (17)	Br1—C17—C18—C19	172.52 (13)
C6—N1—C7—C8	−110.24 (15)	Br1A—C17—C18—C19	179.5 (3)
C2—N1—C7—C8	69.39 (18)	C17—C18—C19—C14	1.1 (2)
C6—N1—C7—C12	68.39 (17)	C15—C14—C19—C18	1.4 (2)
C2—N1—C7—C12	−111.98 (15)	C4—C14—C19—C18	−176.83 (13)

Symmetry code: (i) −*x*+1, *y*, −*z*+1/2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···Br1^{ii}	0.82 (2)	2.75 (2)	3.507 (3)	154.4 (19)
N2—H2*A*···Br1*A*^{ii}	0.82 (2)	2.73 (2)	3.493 (4)	155.1 (19)
N2—H2*B*···N3^{iii}	0.84 (2)	2.24 (2)	3.0583 (18)	165 (2)
C5—H5*B*···N3^{iv}	0.99	2.59	3.5426 (19)	160
C8—H8···O2^{v}	0.95	2.49	3.223 (2)	134
C12—H12···N3^{vi}	0.95	2.65	3.411 (2)	138
C16—H16···N3^{vii}	0.95	2.62	3.5283 (19)	160
O2—H2*C*···O1	0.85 (1)	2.09 (2)	2.8739 (14)	153 (3)

Symmetry codes: (ii) *x*, −*y*+2, *z*+1/2; (iii) −*x*+3/2, −*y*+5/2, −*z*+1; (iv) *x*, *y*−1, *z*; (v) *x*, *y*+1, *z*; (vi) −*x*+3/2, −*y*+3/2, −*z*+1; (vii) −*x*+3/2, *y*−1/2, −*z*+1/2.

1,6-Diamino-2-oxo-4-phenyl-1,2-dihydropyridine-3,5-dicarbonitrile (II)

Crystal data

$C_{13}H_9N_5O$
M_r = 251.25
Triclinic, $P\overline{1}$
a = 8.6444 (1) Å
b = 8.9104 (2) Å
c = 16.0902 (2) Å
α = 79.196 (1)°
β = 86.485 (1)°
γ = 69.003 (2)°
V = 1136.52 (4) Å^3
Z = 4
F(000) = 520
D_x = 1.468 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 60859 reflections
θ = 2.5–35.6°

μ = 0.10 mm^{-1}
T = 100 K

Prism, colourless
0.15 × 0.12 × 0.06 mm

Data collection

XtaLAB Synergy, Dualflex, HyPix diffractometer
Radiation source: micro-focus sealed X-ray tube
φ and ω scans
Absorption correction: multi-scan (CrysAlisPro; Rigaku OD, 2021)
T_{min} = 0.972, T_{max} = 0.980
88754 measured reflections

9666 independent reflections
8561 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 35.4°, θ_{min} = 2.5°
h = −14→13
k = −14→14
l = −25→26

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.118
S = 1.03
9666 reflections
363 parameters
0 restraints

Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0719P)^2 + 0.2449P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.54 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
C2	0.49789 (8)	0.24937 (8)	0.36884 (4)	0.01381 (11)
C3	0.53566 (8)	0.37133 (8)	0.30738 (4)	0.01370 (11)
C4	0.48775 (8)	0.53309 (8)	0.31837 (4)	0.01268 (10)
C5	0.39202 (8)	0.57960 (7)	0.38978 (4)	0.01268 (10)
C6	0.33478 (8)	0.46771 (8)	0.44558 (4)	0.01249 (10)
C7	0.63071 (9)	0.31152 (8)	0.23688 (4)	0.01525 (11)
C8	0.53483 (8)	0.65513 (8)	0.25605 (4)	0.01337 (11)
C9	0.50427 (10)	0.67233 (8)	0.16981 (4)	0.01755 (12)
H9	0.453811	0.605695	0.151080	0.021*
C10	0.54766 (11)	0.78697 (9)	0.11127 (5)	0.02109 (14)
H10	0.526489	0.798239	0.052760	0.025*
C11	0.62188 (10)	0.88513 (9)	0.13807 (5)	0.02022 (13)
H11	0.652279	0.962460	0.097961	0.024*
C12	0.65120 (9)	0.86934 (8)	0.22373 (5)	0.01812 (12)
H12	0.700559	0.937029	0.242277	0.022*
C13	0.60864 (9)	0.75488 (8)	0.28249 (4)	0.01520 (11)
H13	0.629797	0.744330	0.340946	0.018*
C14	0.34605 (8)	0.74045 (8)	0.40775 (4)	0.01414 (11)
N1	0.38849 (7)	0.30955 (7)	0.43300 (4)	0.01336 (10)

N2	0.33246 (8)	0.19935 (7)	0.49062 (4)	0.01632 (11)
H2A	0.3085 (16)	0.1388 (16)	0.4569 (8)	0.027 (3)*
H2B	0.4202 (17)	0.1317 (16)	0.5247 (8)	0.029 (3)*
N3	0.70345 (9)	0.25693 (8)	0.18045 (4)	0.02017 (12)
N4	0.31176 (8)	0.86837 (7)	0.42590 (4)	0.01799 (11)
N5	0.23470 (8)	0.50589 (7)	0.51032 (4)	0.01504 (10)
H5A	0.1960 (17)	0.4294 (17)	0.5378 (8)	0.030 (3)*
H5B	0.1916 (17)	0.6134 (17)	0.5190 (9)	0.031 (3)*
O1	0.55120 (7)	0.10126 (6)	0.36855 (3)	0.01817 (10)
C2′	0.97520 (8)	0.16536 (7)	0.35832 (4)	0.01262 (11)
C3′	1.02820 (8)	0.27412 (7)	0.29632 (4)	0.01245 (10)
C4′	1.08425 (8)	0.23854 (7)	0.21668 (4)	0.01188 (10)
C5′	1.09636 (8)	0.08798 (7)	0.19804 (4)	0.01221 (10)
C6′	1.04791 (8)	−0.02418 (7)	0.25855 (4)	0.01190 (10)
C7′	1.02248 (9)	0.42022 (8)	0.32183 (4)	0.01393 (11)
C8′	1.12573 (5)	0.36189 (4)	0.15294 (3)	0.01286 (11)
C9′	1.00656 (4)	0.51639 (5)	0.13008 (3)	0.01666 (12)
H9′	0.899783	0.541883	0.154979	0.020*
C10′	1.04361 (6)	0.63360 (4)	0.07079 (3)	0.02107 (14)
H10′	0.962158	0.739194	0.055167	0.025*
C11′	1.19983 (6)	0.59630 (5)	0.03436 (3)	0.02295 (15)
H11′	1.225153	0.676408	−0.006158	0.028*
C12′	1.31900 (5)	0.44180 (6)	0.05723 (3)	0.02250 (15)
H12′	1.425776	0.416311	0.032329	0.027*
C13′	1.28195 (5)	0.32459 (4)	0.11652 (3)	0.01777 (12)
H13′	1.363404	0.218998	0.132141	0.021*
C14′	1.14171 (9)	0.04541 (8)	0.11662 (4)	0.01460 (11)
N1′	0.98460 (7)	0.01996 (6)	0.33357 (3)	0.01239 (10)
N2′	0.93299 (8)	−0.09390 (7)	0.39068 (4)	0.01582 (11)
H2A′	0.9758 (16)	−0.1024 (15)	0.4416 (8)	0.022 (3)*
H2B′	0.8215 (18)	−0.0479 (17)	0.3919 (9)	0.032 (3)*
N3′	1.01668 (9)	0.53667 (7)	0.34567 (4)	0.01855 (12)
N4′	1.17585 (9)	0.00229 (8)	0.05229 (4)	0.02098 (12)
N5′	1.05814 (8)	−0.16991 (7)	0.24521 (4)	0.01556 (11)
H5A′	1.0282 (19)	−0.2369 (18)	0.2854 (9)	0.039 (4)*
H5B′	1.0896 (15)	−0.2001 (15)	0.1954 (8)	0.023 (3)*
O1′	0.92331 (7)	0.18943 (6)	0.42983 (3)	0.01749 (10)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C2	0.0160 (3)	0.0122 (2)	0.0135 (2)	−0.0053 (2)	0.0029 (2)	−0.00348 (19)
C3	0.0169 (3)	0.0119 (2)	0.0126 (2)	−0.0055 (2)	0.0032 (2)	−0.00320 (19)
C4	0.0144 (3)	0.0120 (2)	0.0119 (2)	−0.0050 (2)	0.00073 (19)	−0.00226 (18)
C5	0.0156 (3)	0.0106 (2)	0.0122 (2)	−0.0051 (2)	0.00160 (19)	−0.00266 (18)
C6	0.0145 (3)	0.0116 (2)	0.0115 (2)	−0.0046 (2)	0.00057 (19)	−0.00262 (18)
C7	0.0173 (3)	0.0134 (2)	0.0150 (3)	−0.0056 (2)	0.0018 (2)	−0.0027 (2)
C8	0.0160 (3)	0.0117 (2)	0.0121 (2)	−0.0049 (2)	0.00167 (19)	−0.00189 (18)

C9	0.0234 (3)	0.0156 (3)	0.0129 (3)	−0.0059 (2)	−0.0002 (2)	−0.0026 (2)
C10	0.0292 (4)	0.0173 (3)	0.0127 (3)	−0.0047 (3)	0.0022 (2)	−0.0006 (2)
C11	0.0244 (3)	0.0141 (3)	0.0183 (3)	−0.0046 (2)	0.0068 (2)	0.0002 (2)
C12	0.0199 (3)	0.0147 (3)	0.0204 (3)	−0.0078 (2)	0.0051 (2)	−0.0028 (2)
C13	0.0177 (3)	0.0144 (3)	0.0146 (3)	−0.0073 (2)	0.0020 (2)	−0.0025 (2)
C14	0.0156 (3)	0.0135 (2)	0.0138 (2)	−0.0059 (2)	0.0018 (2)	−0.00275 (19)
N1	0.0169 (2)	0.0103 (2)	0.0131 (2)	−0.00544 (18)	0.00382 (18)	−0.00272 (17)
N2	0.0212 (3)	0.0126 (2)	0.0161 (2)	−0.0083 (2)	0.0051 (2)	−0.00171 (18)
N3	0.0222 (3)	0.0194 (3)	0.0181 (3)	−0.0063 (2)	0.0046 (2)	−0.0052 (2)
N4	0.0207 (3)	0.0149 (2)	0.0200 (3)	−0.0077 (2)	0.0039 (2)	−0.0052 (2)
N5	0.0189 (3)	0.0128 (2)	0.0133 (2)	−0.00552 (19)	0.00438 (19)	−0.00362 (17)
O1	0.0235 (2)	0.0112 (2)	0.0197 (2)	−0.00596 (18)	0.00526 (19)	−0.00440 (16)
C2′	0.0176 (3)	0.0089 (2)	0.0115 (2)	−0.0048 (2)	0.00219 (19)	−0.00237 (18)
C3′	0.0179 (3)	0.0091 (2)	0.0115 (2)	−0.0061 (2)	0.00252 (19)	−0.00242 (18)
C4′	0.0144 (3)	0.0097 (2)	0.0116 (2)	−0.00459 (19)	0.00144 (19)	−0.00171 (18)
C5′	0.0168 (3)	0.0100 (2)	0.0101 (2)	−0.0053 (2)	0.00269 (19)	−0.00226 (18)
C6′	0.0149 (3)	0.0095 (2)	0.0115 (2)	−0.00460 (19)	0.00159 (19)	−0.00249 (18)
C7′	0.0186 (3)	0.0113 (2)	0.0123 (2)	−0.0063 (2)	0.0015 (2)	−0.00144 (19)
C8′	0.0178 (3)	0.0108 (2)	0.0112 (2)	−0.0070 (2)	0.00243 (19)	−0.00177 (18)
C9′	0.0212 (3)	0.0126 (2)	0.0142 (3)	−0.0052 (2)	0.0010 (2)	0.0004 (2)
C10′	0.0331 (4)	0.0148 (3)	0.0148 (3)	−0.0099 (3)	−0.0004 (3)	0.0017 (2)
C11′	0.0400 (4)	0.0200 (3)	0.0153 (3)	−0.0195 (3)	0.0056 (3)	−0.0022 (2)
C12′	0.0300 (4)	0.0217 (3)	0.0226 (3)	−0.0175 (3)	0.0122 (3)	−0.0076 (3)
C13′	0.0199 (3)	0.0152 (3)	0.0208 (3)	−0.0094 (2)	0.0068 (2)	−0.0051 (2)
C14′	0.0190 (3)	0.0113 (2)	0.0133 (2)	−0.0057 (2)	0.0020 (2)	−0.00160 (19)
N1′	0.0184 (2)	0.0086 (2)	0.0109 (2)	−0.00621 (18)	0.00355 (17)	−0.00196 (16)
N2′	0.0235 (3)	0.0116 (2)	0.0138 (2)	−0.0093 (2)	0.0063 (2)	−0.00122 (17)
N3′	0.0277 (3)	0.0133 (2)	0.0168 (2)	−0.0098 (2)	0.0017 (2)	−0.00329 (19)
N4′	0.0300 (3)	0.0178 (3)	0.0148 (2)	−0.0079 (2)	0.0039 (2)	−0.0045 (2)
N5′	0.0239 (3)	0.0105 (2)	0.0146 (2)	−0.0085 (2)	0.0047 (2)	−0.00454 (18)
O1′	0.0286 (3)	0.0125 (2)	0.0116 (2)	−0.00763 (18)	0.00628 (18)	−0.00403 (15)

Geometric parameters (Å, º)

C2—O1	1.2330 (8)	C2′—O1′	1.2376 (7)
C2—N1	1.4044 (8)	C2′—N1′	1.3992 (8)
C2—C3	1.4412 (9)	C2′—C3′	1.4296 (8)
C3—C4	1.3925 (9)	C3′—C4′	1.3939 (9)
C3—C7	1.4300 (9)	C3′—C7′	1.4204 (9)
C4—C5	1.4117 (9)	C4′—C5′	1.3954 (8)
C4—C8	1.4872 (9)	C4′—C8′	1.4843
C5—C6	1.4172 (9)	C5′—C6′	1.4167 (8)
C5—C14	1.4243 (9)	C5′—C14′	1.4251 (9)
C6—N5	1.3268 (8)	C6′—N5′	1.3266 (8)
C6—N1	1.3672 (8)	C6′—N1′	1.3617 (8)
C7—N3	1.1545 (9)	C7′—N3′	1.1558 (8)
C8—C9	1.3982 (9)	C8′—C9′	1.3900
C8—C13	1.3999 (9)	C8′—C13′	1.3900

C9—C10	1.3935 (10)	C9′—C10′	1.3900
C9—H9	0.9500	C9′—H9′	0.9500
C10—C11	1.3928 (12)	C10′—C11′	1.3900
C10—H10	0.9500	C10′—H10′	0.9500
C11—C12	1.3887 (11)	C11′—C12′	1.3900
C11—H11	0.9500	C11′—H11′	0.9500
C12—C13	1.3907 (9)	C12′—C13′	1.3900
C12—H12	0.9500	C12′—H12′	0.9500
C13—H13	0.9500	C13′—H13′	0.9500
C14—N4	1.1595 (9)	C14′—N4′	1.1561 (9)
N1—N2	1.4151 (8)	N1′—N2′	1.4132 (7)
N2—H2A	0.913 (13)	N2′—H2A′	0.898 (13)
N2—H2B	0.916 (14)	N2′—H2B′	0.902 (15)
N5—H5A	0.897 (14)	N5′—H5A′	0.887 (15)
N5—H5B	0.930 (14)	N5′—H5B′	0.889 (12)
O1—C2—N1	118.98 (6)	O1′—C2′—N1′	118.89 (6)
O1—C2—C3	125.76 (6)	O1′—C2′—C3′	125.90 (6)
N1—C2—C3	115.25 (5)	N1′—C2′—C3′	115.20 (5)
C4—C3—C7	123.26 (6)	C4′—C3′—C7′	122.09 (6)
C4—C3—C2	121.92 (6)	C4′—C3′—C2′	122.48 (5)
C7—C3—C2	114.77 (5)	C7′—C3′—C2′	115.42 (5)
C3—C4—C5	118.58 (6)	C3′—C4′—C5′	118.84 (5)
C3—C4—C8	120.96 (6)	C3′—C4′—C8′	119.79 (5)
C5—C4—C8	120.46 (5)	C5′—C4′—C8′	121.35 (5)
C4—C5—C6	120.81 (6)	C4′—C5′—C6′	120.19 (5)
C4—C5—C14	121.79 (6)	C4′—C5′—C14′	122.74 (6)
C6—C5—C14	117.38 (6)	C6′—C5′—C14′	116.82 (5)
N5—C6—N1	117.80 (6)	N5′—C6′—N1′	117.96 (6)
N5—C6—C5	124.17 (6)	N5′—C6′—C5′	123.20 (6)
N1—C6—C5	118.01 (6)	N1′—C6′—C5′	118.83 (5)
N3—C7—C3	176.29 (7)	N3′—C7′—C3′	177.41 (7)
C9—C8—C13	119.10 (6)	C9′—C8′—C13′	120.0
C9—C8—C4	120.01 (6)	C9′—C8′—C4′	119.3
C13—C8—C4	120.89 (6)	C13′—C8′—C4′	120.7
C10—C9—C8	120.16 (7)	C8′—C9′—C10′	120.0
C10—C9—H9	119.9	C8′—C9′—H9′	120.0
C8—C9—H9	119.9	C10′—C9′—H9′	120.0
C11—C10—C9	120.37 (7)	C11′—C10′—C9′	120.0
C11—C10—H10	119.8	C11′—C10′—H10′	120.0
C9—C10—H10	119.8	C9′—C10′—H10′	120.0
C12—C11—C10	119.63 (6)	C10′—C11′—C12′	120.0
C12—C11—H11	120.2	C10′—C11′—H11′	120.0
C10—C11—H11	120.2	C12′—C11′—H11′	120.0
C11—C12—C13	120.31 (7)	C13′—C12′—C11′	120.0
C11—C12—H12	119.8	C13′—C12′—H12′	120.0
C13—C12—H12	119.8	C11′—C12′—H12′	120.0
C12—C13—C8	120.42 (6)	C12′—C13′—C8′	120.0

C12—C13—H13	119.8	C12′—C13′—H13′	120.0
C8—C13—H13	119.8	C8′—C13′—H13′	120.0
N4—C14—C5	176.96 (7)	N4′—C14′—C5′	175.70 (7)
C6—N1—C2	124.55 (5)	C6′—N1′—C2′	124.25 (5)
C6—N1—N2	116.97 (5)	C6′—N1′—N2′	116.70 (5)
C2—N1—N2	118.46 (5)	C2′—N1′—N2′	118.98 (5)
N1—N2—H2A	103.6 (8)	N1′—N2′—H2A′	107.0 (8)
N1—N2—H2B	107.6 (8)	N1′—N2′—H2B′	104.9 (9)
H2A—N2—H2B	108.0 (11)	H2A′—N2′—H2B′	110.0 (12)
C6—N5—H5A	117.0 (9)	C6′—N5′—H5A′	120.0 (10)
C6—N5—H5B	119.9 (8)	C6′—N5′—H5B′	121.0 (8)
H5A—N5—H5B	122.0 (12)	H5A′—N5′—H5B′	118.9 (12)
O1—C2—C3—C4	−171.43 (7)	O1′—C2′—C3′—C4′	−179.57 (7)
N1—C2—C3—C4	9.53 (10)	N1′—C2′—C3′—C4′	0.40 (10)
O1—C2—C3—C7	6.26 (10)	O1′—C2′—C3′—C7′	1.41 (10)
N1—C2—C3—C7	−172.78 (6)	N1′—C2′—C3′—C7′	−178.62 (6)
C7—C3—C4—C5	179.14 (6)	C7′—C3′—C4′—C5′	175.94 (6)
C2—C3—C4—C5	−3.36 (10)	C2′—C3′—C4′—C5′	−3.01 (10)
C7—C3—C4—C8	−0.34 (10)	C7′—C3′—C4′—C8′	−5.56 (10)
C2—C3—C4—C8	177.16 (6)	C2′—C3′—C4′—C8′	175.49 (6)
C3—C4—C5—C6	−4.87 (10)	C3′—C4′—C5′—C6′	1.73 (10)
C8—C4—C5—C6	174.61 (6)	C8′—C4′—C5′—C6′	−176.75 (5)
C3—C4—C5—C14	176.52 (6)	C3′—C4′—C5′—C14′	175.69 (6)
C8—C4—C5—C14	−3.99 (10)	C8′—C4′—C5′—C14′	−2.79 (10)
C4—C5—C6—N5	−174.96 (6)	C4′—C5′—C6′—N5′	−179.18 (6)
C14—C5—C6—N5	3.70 (10)	C14′—C5′—C6′—N5′	6.51 (10)
C4—C5—C6—N1	6.35 (9)	C4′—C5′—C6′—N1′	2.15 (10)
C14—C5—C6—N1	−174.99 (6)	C14′—C5′—C6′—N1′	−172.16 (6)
C3—C4—C8—C9	50.86 (9)	C3′—C4′—C8′—C9′	−56.14 (7)
C5—C4—C8—C9	−128.61 (7)	C5′—C4′—C8′—C9′	122.33 (6)
C3—C4—C8—C13	−129.66 (7)	C3′—C4′—C8′—C13′	123.55 (6)
C5—C4—C8—C13	50.87 (9)	C5′—C4′—C8′—C13′	−57.99 (7)
C13—C8—C9—C10	0.27 (10)	C13′—C8′—C9′—C10′	0.0
C4—C8—C9—C10	179.76 (6)	C4′—C8′—C9′—C10′	179.7
C8—C9—C10—C11	0.08 (11)	C8′—C9′—C10′—C11′	0.0
C9—C10—C11—C12	−0.60 (12)	C9′—C10′—C11′—C12′	0.0
C10—C11—C12—C13	0.77 (11)	C10′—C11′—C12′—C13′	0.0
C11—C12—C13—C8	−0.43 (11)	C11′—C12′—C13′—C8′	0.0
C9—C8—C13—C12	−0.10 (10)	C9′—C8′—C13′—C12′	0.0
C4—C8—C13—C12	−179.58 (6)	C4′—C8′—C13′—C12′	−179.7
N5—C6—N1—C2	−178.25 (6)	N5′—C6′—N1′—C2′	176.16 (6)
C5—C6—N1—C2	0.53 (10)	C5′—C6′—N1′—C2′	−5.10 (10)
N5—C6—N1—N2	−0.09 (9)	N5′—C6′—N1′—N2′	−0.78 (9)
C5—C6—N1—N2	178.69 (6)	C5′—C6′—N1′—N2′	177.97 (6)
O1—C2—N1—C6	172.72 (7)	O1′—C2′—N1′—C6′	−176.24 (6)
C3—C2—N1—C6	−8.16 (10)	C3′—C2′—N1′—C6′	3.79 (10)
O1—C2—N1—N2	−5.41 (10)	O1′—C2′—N1′—N2′	0.63 (10)

C3—C2—N1—N2	173.70 (6)	C3′—C2′—N1′—N2′	−179.34 (6)

Hydrogen-bond geometry (Å, º)

*Cg*2 is the centroid of the C8–C13 phenyl ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···N4^{i}	0.913 (13)	2.541 (13)	3.3713 (9)	151.6 (11)
N2—H2*B*···N4^{ii}	0.916 (14)	2.495 (14)	3.2404 (10)	138.7 (11)
N2—H2*B*···O1^{iii}	0.916 (14)	2.381 (13)	3.0650 (8)	131.5 (11)
N5—H5*A*···N3′^{ii}	0.897 (14)	2.525 (14)	3.1431 (9)	126.6 (11)
N5—H5*B*···O1′^{ii}	0.930 (14)	1.986 (14)	2.8853 (8)	162.3 (12)
N2′—H2*A*′···O1′^{iv}	0.898 (13)	2.186 (13)	3.0608 (8)	164.4 (11)
N2′—H2*B*′···N2^{iii}	0.902 (15)	2.681 (14)	3.1829 (8)	116.1 (10)
N2′—H2*B*′···O1	0.902 (15)	2.250 (15)	3.1373 (9)	167.5 (12)
N5′—H5*A*′···N3′^{i}	0.887 (15)	2.102 (15)	2.9314 (8)	155.2 (13)
C9′—H9′···*Cg*2	0.95	2.93	3.7972 (5)	153

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