

Hydrogen-bonding patterns in the cocrystal 2-amino-4,6-dimethoxy-pyrimidine–anthranilic acid (1/1)

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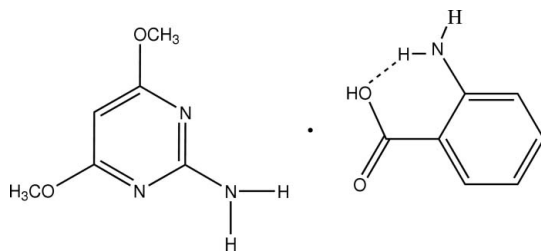
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Key indicators: single-crystal X-ray study; $T = 120$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.050; wR factor = 0.134; data-to-parameter ratio = 16.1.

In the title cocrystal, $\text{C}_6\text{H}_9\text{N}_3\text{O}_2 \cdot \text{C}_7\text{H}_7\text{NO}_2$, the asymmetric unit contains two crystallographically independent 2-amino-4,6-dimethoxy pyrimidine–anthranilic acid adducts. The 2-amino-4,6-dimethoxy pyrimidine molecules interact with the carboxylic group of the respective anthranilic acid molecules through $\text{N}-\text{H} \cdots \text{O}$ and $\text{O}-\text{H} \cdots \text{N}$ hydrogen bonds, forming a cyclic hydrogen-bonded motif $R_2^2(8)$. The pyrimidine molecules also form base pairs *via* a pair of $\text{N}-\text{H} \cdots \text{N}$ hydrogen bonds, forming another $R_2^2(8)$ motif. The typical intramolecular $\text{N}-\text{H} \cdots \text{O}$ hydrogen bond is observed in the anthranilic acid molecules. Furthermore, the crystal structure is stabilized by $\text{C}-\text{H} \cdots \text{O}$ hydrogen bonds.

Related literature

For related literature, see: Baker & Santi (1965); Balasubramani *et al.* (2005, 2006); Bernstein *et al.* (1995); Boone *et al.* (1977); Chinnakali *et al.* (1999); Desiraju (1989); Etter (1990); Hunt *et al.* (1980); Hunter (1994); Low *et al.* (2002); Lynch & Jones (2004); Muthiah *et al.* (2006); Schwalbe & Williams (1982); Stanley *et al.* (2005); Takazawa *et al.* (1986); Thanigaimani *et al.* (2006, 2007a,b).



Experimental

Crystal data

$\text{C}_6\text{H}_9\text{N}_3\text{O}_2 \cdot \text{C}_7\text{H}_7\text{NO}_2$
 $M_r = 292.30$
 Triclinic, $P\bar{1}$
 $a = 7.2802$ (3) Å
 $b = 7.4095$ (2) Å
 $c = 25.8035$ (9) Å
 $\alpha = 83.636$ (2)°
 $\beta = 83.1620$ (10)°

$\gamma = 82.373$ (2)°
 $V = 1363.38$ (8) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.11$ mm⁻¹
 $T = 120$ K
 $0.24 \times 0.19 \times 0.08$ mm

Data collection

Bruker–Nonius KappaCCD diffractometer
 Absorption correction: none
 24443 measured reflections

6286 independent reflections
 4140 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.064$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.050$
 $wR(F^2) = 0.134$
 $S = 1.04$
 6286 reflections
 390 parameters

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.29$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.31$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$\text{N2A}-\text{H2A1} \cdots \text{O4A}$	0.86	1.97	2.818 (2)	169
$\text{N2A}-\text{H2A2} \cdots \text{N3A}^{\text{i}}$	0.86	2.35	3.166 (2)	160
$\text{O3A}-\text{H3A} \cdots \text{N1A}$	0.82	1.86	2.6808 (19)	175
$\text{O4B}-\text{H4B} \cdots \text{N1B}$	0.82	1.81	2.603 (2)	164
$\text{N4A}-\text{H7} \cdots \text{O4A}$	0.91 (2)	1.97 (2)	2.650 (2)	130 (2)
$\text{N2B}-\text{H2B1} \cdots \text{O3B}$	0.86	2.22	3.075 (2)	170
$\text{N2B}-\text{H2B2} \cdots \text{N3B}^{\text{ii}}$	0.86	2.33	3.165 (2)	164
$\text{N4A}-\text{H16} \cdots \text{N4A}^{\text{iii}}$	0.87 (2)	2.58 (2)	3.100 (3)	119.7 (18)
$\text{N4B}-\text{H4B1} \cdots \text{O3B}$	0.86	2.12	2.749 (2)	129
$\text{N4B}-\text{H4B2} \cdots \text{O3A}^{\text{iv}}$	0.86	2.59	3.450 (2)	176
$\text{C8B}-\text{H8B3} \cdots \text{O3B}^{\text{iv}}$	0.96	2.47	3.339 (2)	150
$\text{C14A}-\text{H14A} \cdots \text{O3A}$	0.93	2.42	2.747 (3)	100
$\text{C14B}-\text{H14B} \cdots \text{O4B}$	0.93	2.30	2.655 (2)	102

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

Data collection: *COLLECT* (Hooft, 1998); cell refinement: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2644).

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supporting information

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Hydrogen-bonding patterns in the cocrystal 2-amino-4,6-dimethoxypyrimidine–anthranilic acid (1/1)

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S1. Comment

Aminopyrimidine-Carboxylate interactions are of fundamental importance since they are involved in protein-nucleic acids recognition and protein-drug binding (Hunt *et al.*, 1980; Baker & Santi, 1965). Hydrogen bonding plays a key role in molecular recognition and crystal engineering research (Desiraju, 1989). The adducts of carboxylic acids with 2-aminoheterocyclic ring system form a graph-set motif $R_2^2(8)$ (Lynch & Jones, 2004). This motif is very robust in aminopyrimidine-carboxylic acid/ carboxylates systems. The crystal structures of aminopyrimidine derivatives (Schwalbe & Williams, 1982), aminopyrimidine carboxylates (Stanley *et al.*, 2005) and co-crystals (Chinnakali *et al.*, 1999) have been reported. The crystal structure of 2-amino-4,6-dimethoxy pyrimidine has also been reported (Low *et al.*, 2002). The crystal structures of 2-amino-4,6-dimethoxy pyrimidine 4-aminobenzoic acid (1/1) (Thanigaimani *et al.*, 2006), 2-amino-4,6-dimethoxy pyrimidine phthalic acid (1/1) (Thanigaimani *et al.*, 2007a), 2-amino-4,6-dimethyl pyrimidine cinnamic acid (1/2) (Balasubramani *et al.*, 2005) and 2-amino-4,6-dimethyl pyrimidine 4-hydroxybenzoic acid (1/1) (Balasubramani *et al.*, 2006), have been recently reported from our laboratory. The crystal structure of anthranilic acid (Boone *et al.*, 1977; Takazawa *et al.*, 1986) is known. In the present study, the hydrogen-bonding patterns in the 2-amino-4,6-dimethoxypyrimidine anthranilic acid (1/1) cocrystal, (I), are investigated.

The asymmetric unit (Fig. 1) contains pair of molecules of 2-amino-4,6-dimethoxypyrimidine (A&B) and anthranilic acid (A&B). The carboxyl group of each anthranilic acid interacts with the corresponding 2-amino-4,6-dimethoxy pyrimidine molecule *via* a pair of N—H···O and O—H···N hydrogen bonds generating $R_2^2(8)$ ring motif. (Etter, 1990; Bernstein *et al.*, 1995). In both the types (A & B) inversion related bases are paired *via* (2) N—H···N(3) hydrogen bonds forming another type of $R_2^2(8)$ motif. This type of base pairing has been reported in the crystal structures of 2-amino-4,6-dimethylpyrimidinium salicylate (Muthiah *et al.*, 2006) and 2-amino-4,6-dimethoxypyrimidinium 4-hydroxybenzoate (Thanigaimani *et al.*, 2007b). The carboxyl oxygen atom (O3A) of anthranilic acid (Molecule A) is linked to 4-amino group (N4B) of anthranilic acid (Molecule B) *via* N—H···O hydrogen bonds. In each of the anthranilic acid molecule, there is a typical intramolecular hydrogen bond between the amino NH₂ group and the carboxylic group, (graph-set notation S6). There is also a C—H···O hydrogen bond involving atom C8B of the pyrimidine moiety and O4B of the anthranilic acid molecule. The π - π stacking interactions between the aromatic ring are also observed. The pyrimidine ring of 2-amino-4,6-dimethoxy pyrimidine (molecule A) forms stacking interactions with the aryl rings of the anthranilic acid (molecule A), with interplanar and centroid-centroid distance of 3.430 Å and 3.5436 (11) Å, respectively, and a slip angle (angle between the centroid vector and the normal to the plane) is 13.85°. A similar type of stacking is also observed between two 2-amino-4,6-dimethoxy pyrimidine (molecule B) related by an inversion centre. The centroid-centroid distance and interplanar distance are 3.5411 (10) Å and 3.380 Å, respectively, the slip angle being 17.33°. These are typical aromatic stacking values (Hunter, 1994).

S2. Experimental

A hot methanol solution (20 ml) of 2-amino-4,6-dimethoxypyrimidine (38 mg, Aldrich) and anthranilic acid (34 mg, Loba Chemie) was warmed for half an hour over a water bath. The mixture was cooled slowly and kept at room temperature; after a few days, colourless plate-like crystals were obtained.

S3. Refinement

The hydrogen atoms of the N4A (H4A1, H4A2) were located in difference Fourier map and refined freely. The other hydrogen atoms were positioned geometrically and were refined using a riding model. The C—H and O—H bond lengths are 0.93–0.96 and 0.82 Å respectively [$U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C}, \text{O})$].

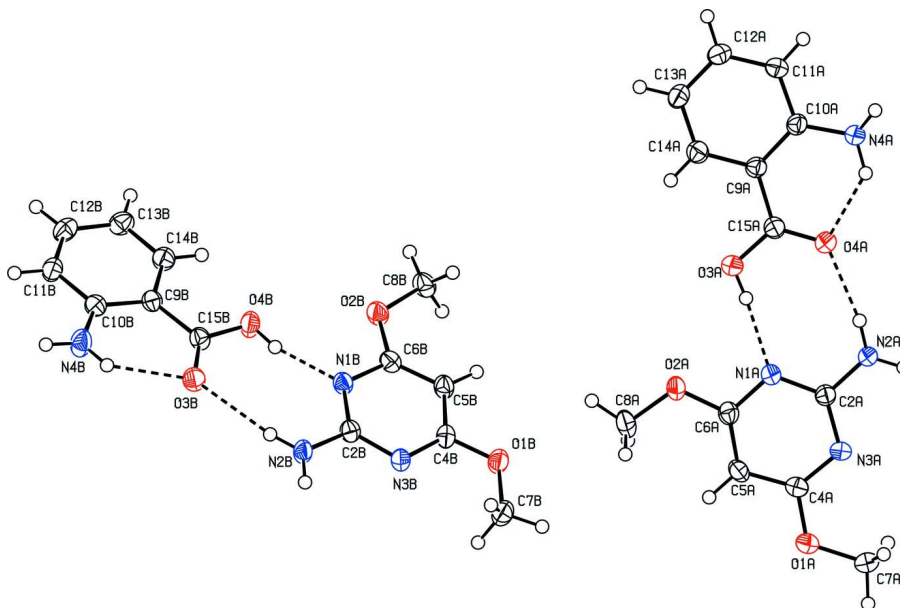


Figure 1

The asymmetric unit of (I), showing 50% probability displacement ellipsoids. Dashed lines indicate hydrogen bonds.

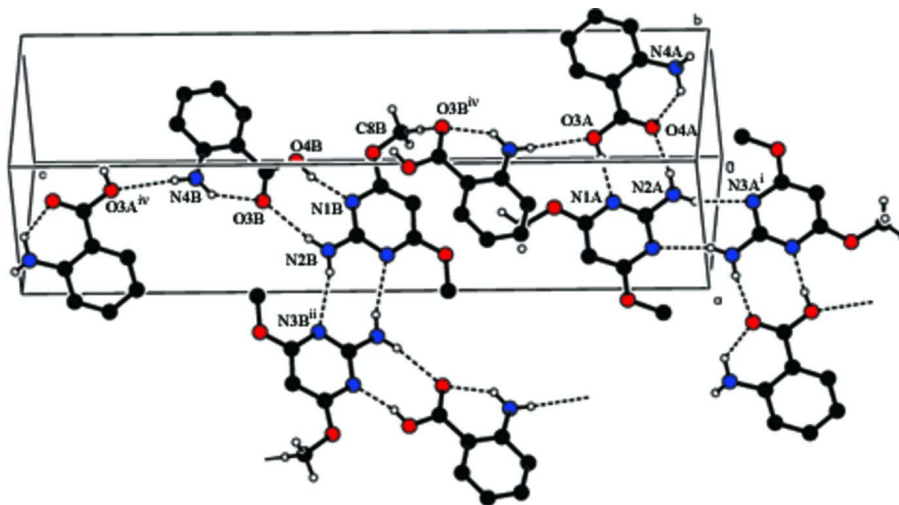


Figure 2

The crystal structure of (I). Dashed lines indicate hydrogen bonds [symmetry code: (i) $-x + 2, -y + 1, -z$; (ii) $-x + 3, -y + 1, -z + 1$; (iv) $-x + 2, -y + 2, -z + 1$].

2-amino-4,6-dimethoxypyrimidine–anthranilic acid (1/1)

Crystal data

C₆H₉N₃O₂·C₇H₇NO₂ $M_r = 292.30$ Triclinic, $P\bar{1}$

Hall symbol: -P 1

 $a = 7.2802 (3) \text{ \AA}$ $b = 7.4095 (2) \text{ \AA}$ $c = 25.8035 (9) \text{ \AA}$ $\alpha = 83.636 (2)^\circ$ $\beta = 83.162 (1)^\circ$ $\gamma = 82.373 (2)^\circ$ $V = 1363.38 (8) \text{ \AA}^3$ $Z = 4$ $F(000) = 616$ $D_x = 1.424 \text{ Mg m}^{-3}$ Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 25 reflections

 $\theta = 3.0\text{--}27.6^\circ$ $\mu = 0.11 \text{ mm}^{-1}$ $T = 120 \text{ K}$

Plate-like, colourless

 $0.24 \times 0.19 \times 0.08 \text{ mm}$

Data collection

Bruker–Nonius CCD

diffractometer

Radiation source: Bruker–Nonius FR591

rotating anode

Graphite monochromator

Detector resolution: $9.091 \text{ pixels mm}^{-1}$ φ and ω scans

24443 measured reflections

6286 independent reflections

4140 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.064$ $\theta_{\text{max}} = 27.6^\circ$, $\theta_{\text{min}} = 3.0^\circ$ $h = -9 \rightarrow 9$ $k = -9 \rightarrow 9$ $l = -33 \rightarrow 33$

Refinement

Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.050$ $wR(F^2) = 0.134$ $S = 1.04$

6286 reflections

390 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

 $w = 1/[\sigma^2(F_o^2) + (0.0585P)^2 + 0.223P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\text{max}} = 0.001$ $\Delta\rho_{\text{max}} = 0.29 \text{ e \AA}^{-3}$ $\Delta\rho_{\text{min}} = -0.31 \text{ e \AA}^{-3}$ Extinction correction: *SHELXL*, $FC^* = KFC[1 + 0.001XFC^2\Lambda^3/\text{SIN}(2\Theta)]^{-1/4}$

Extinction coefficient: 0.022 (3)

Special details

Geometry. Bond distances, angles *etc.* have been calculated using the rounded fractional coordinates. All e.s.d.'s are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted R -factors wR and all goodnesses 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 observed criterion of $F^2 > \sigma(F^2)$ is used only for calculating $-R$ -factor-obs *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	$U_{\text{iso}}^*/U_{\text{eq}}$
O1A	1.21498 (19)	0.13688 (17)	0.11198 (5)	0.0321 (4)
O2A	0.9788 (2)	0.62312 (17)	0.21411 (5)	0.0325 (4)

N1A	0.9714 (2)	0.65251 (19)	0.12796 (6)	0.0245 (5)
N2A	0.9553 (2)	0.6942 (2)	0.03985 (6)	0.0299 (5)
N3A	1.0875 (2)	0.41201 (19)	0.07324 (6)	0.0242 (5)
C2A	1.0060 (2)	0.5827 (2)	0.08148 (7)	0.0240 (6)
C4A	1.1324 (2)	0.3082 (2)	0.11596 (7)	0.0251 (6)
C5A	1.0999 (3)	0.3628 (2)	0.16628 (7)	0.0282 (6)
C6A	1.0193 (3)	0.5400 (2)	0.16970 (7)	0.0258 (6)
C7A	1.2546 (3)	0.0744 (3)	0.06061 (8)	0.0364 (7)
C8A	1.0194 (3)	0.5193 (3)	0.26230 (7)	0.0425 (8)
O1B	1.23977 (18)	0.52942 (18)	0.36928 (5)	0.0318 (4)
O2B	0.76374 (17)	0.84403 (18)	0.47739 (5)	0.0303 (4)
N1B	1.0400 (2)	0.7436 (2)	0.50440 (6)	0.0250 (5)
N2B	1.3186 (2)	0.6512 (2)	0.53585 (6)	0.0290 (5)
N3B	1.2895 (2)	0.5829 (2)	0.45247 (5)	0.0244 (5)
C2B	1.2140 (3)	0.6598 (2)	0.49642 (7)	0.0244 (6)
C4B	1.1779 (3)	0.5992 (2)	0.41485 (7)	0.0243 (6)
C5B	0.9958 (3)	0.6842 (2)	0.41835 (7)	0.0268 (6)
C6B	0.9336 (3)	0.7556 (2)	0.46478 (7)	0.0251 (6)
C7B	1.4261 (3)	0.4377 (3)	0.36371 (8)	0.0355 (7)
C8B	0.6364 (3)	0.8702 (3)	0.43854 (7)	0.0309 (6)
O3A	0.79403 (19)	0.97701 (17)	0.15298 (5)	0.0306 (4)
O4A	0.7717 (2)	1.03505 (17)	0.06735 (5)	0.0372 (4)
N4A	0.6470 (2)	1.3700 (3)	0.02930 (6)	0.0298 (5)
C9A	0.6511 (2)	1.2676 (2)	0.12255 (7)	0.0240 (5)
C10A	0.6112 (2)	1.4017 (2)	0.08103 (7)	0.0251 (6)
C11A	0.5288 (3)	1.5756 (3)	0.09344 (7)	0.0290 (6)
C12A	0.4867 (3)	1.6146 (3)	0.14425 (7)	0.0315 (6)
C13A	0.5262 (3)	1.4836 (3)	0.18544 (8)	0.0321 (6)
C14A	0.6066 (3)	1.3120 (3)	0.17417 (7)	0.0279 (6)
C15A	0.7426 (3)	1.0846 (2)	0.11184 (7)	0.0259 (6)
O3B	1.10809 (18)	0.82786 (17)	0.63163 (5)	0.0302 (4)
O4B	0.85924 (18)	0.8829 (2)	0.58677 (5)	0.0333 (5)
N4B	1.0645 (2)	0.9650 (2)	0.72764 (6)	0.0355 (6)
C9B	0.8187 (3)	0.9691 (2)	0.67164 (7)	0.0243 (5)
C10B	0.8820 (3)	0.9998 (2)	0.71877 (7)	0.0251 (6)
C11B	0.7504 (3)	1.0696 (3)	0.75827 (7)	0.0293 (6)
C12B	0.5670 (3)	1.1126 (3)	0.75049 (8)	0.0313 (6)
C13B	0.5050 (3)	1.0903 (3)	0.70327 (8)	0.0315 (6)
C14B	0.6303 (3)	1.0186 (3)	0.66481 (7)	0.0300 (6)
C15B	0.9429 (3)	0.8870 (2)	0.62876 (7)	0.0258 (6)
H2A1	0.90370	0.80380	0.04380	0.0360*
H2A2	0.97430	0.65630	0.00910	0.0360*
H7A1	1.31410	-0.04940	0.06330	0.0550*
H7A2	1.33590	0.15120	0.03920	0.0550*
H7A3	1.14050	0.07980	0.04500	0.0550*
H5A	1.13060	0.28490	0.19560	0.0340*
H8A1	0.98330	0.59430	0.29070	0.0640*
H8A2	1.15070	0.47900	0.26080	0.0640*

H8A3	0.95170	0.41500	0.26780	0.0640*
H5B	0.92150	0.69200	0.39110	0.0320*
H2B1	1.27320	0.69810	0.56440	0.0350*
H2B2	1.43160	0.59880	0.53280	0.0350*
H8B1	0.52000	0.93280	0.45240	0.0460*
H8B2	0.61650	0.75350	0.42880	0.0460*
H8B3	0.68700	0.94200	0.40820	0.0460*
H7B1	1.45250	0.39360	0.32970	0.0530*
H7B2	1.43830	0.33640	0.39020	0.0530*
H7B3	1.51240	0.52150	0.36750	0.0530*
H3A	0.84810	0.88000	0.14350	0.0460*
H7	0.722 (3)	1.265 (3)	0.0224 (9)	0.057 (7)*
H11A	0.50220	1.66620	0.06650	0.0350*
H12A	0.43080	1.73080	0.15140	0.0380*
H13A	0.49890	1.51140	0.22000	0.0390*
H14A	0.63210	1.22300	0.20160	0.0330*
H16	0.653 (3)	1.465 (3)	0.0067 (9)	0.046 (7)*
H4B	0.93260	0.83400	0.56440	0.0500*
H11B	0.78900	1.08660	0.79030	0.0350*
H12B	0.48240	1.15760	0.77730	0.0380*
H13B	0.38060	1.12330	0.69780	0.0380*
H14B	0.58890	1.00230	0.63310	0.0360*
H4B1	1.14640	0.92230	0.70380	0.0430*
H4B2	1.09790	0.98560	0.75710	0.0430*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1A	0.0400 (8)	0.0249 (7)	0.0303 (7)	0.0042 (6)	-0.0089 (6)	-0.0023 (6)
O2A	0.0483 (9)	0.0293 (7)	0.0203 (7)	-0.0006 (6)	-0.0080 (6)	-0.0041 (5)
N1A	0.0279 (8)	0.0238 (8)	0.0213 (8)	-0.0010 (6)	-0.0036 (6)	-0.0018 (6)
N2A	0.0427 (10)	0.0238 (8)	0.0205 (8)	0.0073 (7)	-0.0042 (7)	-0.0035 (6)
N3A	0.0249 (8)	0.0212 (8)	0.0255 (8)	0.0018 (6)	-0.0041 (6)	-0.0016 (6)
C2A	0.0226 (10)	0.0262 (10)	0.0230 (9)	-0.0018 (8)	-0.0023 (7)	-0.0027 (7)
C4A	0.0241 (10)	0.0220 (9)	0.0292 (10)	-0.0020 (8)	-0.0055 (8)	-0.0005 (8)
C5A	0.0337 (11)	0.0274 (10)	0.0234 (10)	-0.0018 (8)	-0.0092 (8)	0.0024 (8)
C6A	0.0273 (10)	0.0277 (10)	0.0238 (10)	-0.0052 (8)	-0.0055 (8)	-0.0037 (8)
C7A	0.0461 (13)	0.0269 (10)	0.0337 (11)	0.0092 (9)	-0.0060 (9)	-0.0063 (8)
C8A	0.0650 (16)	0.0404 (13)	0.0218 (10)	-0.0009 (11)	-0.0123 (10)	0.0003 (9)
O1B	0.0296 (7)	0.0409 (8)	0.0255 (7)	0.0022 (6)	-0.0056 (6)	-0.0106 (6)
O2B	0.0225 (7)	0.0416 (8)	0.0264 (7)	0.0017 (6)	-0.0062 (5)	-0.0037 (6)
N1B	0.0224 (8)	0.0311 (9)	0.0214 (8)	-0.0019 (7)	-0.0042 (6)	-0.0022 (6)
N2B	0.0230 (8)	0.0428 (10)	0.0212 (8)	0.0038 (7)	-0.0053 (6)	-0.0088 (7)
N3B	0.0252 (8)	0.0281 (8)	0.0202 (8)	-0.0037 (6)	-0.0026 (6)	-0.0028 (6)
C2B	0.0236 (10)	0.0272 (10)	0.0224 (9)	-0.0053 (8)	-0.0017 (7)	-0.0008 (7)
C4B	0.0282 (10)	0.0265 (10)	0.0194 (9)	-0.0078 (8)	-0.0020 (7)	-0.0030 (7)
C5B	0.0256 (10)	0.0333 (11)	0.0226 (9)	-0.0037 (8)	-0.0062 (7)	-0.0037 (8)
C6B	0.0228 (10)	0.0278 (10)	0.0243 (10)	-0.0032 (8)	-0.0036 (7)	0.0011 (8)

C7B	0.0308 (11)	0.0460 (12)	0.0298 (11)	0.0033 (9)	-0.0038 (8)	-0.0136 (9)
C8B	0.0242 (10)	0.0394 (11)	0.0296 (10)	-0.0029 (9)	-0.0080 (8)	-0.0007 (8)
O3A	0.0376 (8)	0.0260 (7)	0.0255 (7)	0.0048 (6)	-0.0033 (6)	-0.0013 (5)
O4A	0.0541 (9)	0.0290 (7)	0.0252 (7)	0.0094 (7)	-0.0050 (6)	-0.0049 (6)
N4A	0.0387 (10)	0.0255 (9)	0.0225 (9)	0.0059 (8)	-0.0037 (7)	-0.0023 (7)
C9A	0.0210 (9)	0.0260 (9)	0.0248 (9)	-0.0010 (8)	-0.0025 (7)	-0.0040 (7)
C10A	0.0217 (10)	0.0297 (10)	0.0241 (10)	0.0003 (8)	-0.0034 (7)	-0.0064 (8)
C11A	0.0292 (11)	0.0270 (10)	0.0299 (10)	0.0039 (8)	-0.0072 (8)	-0.0029 (8)
C12A	0.0324 (11)	0.0279 (10)	0.0336 (11)	0.0043 (8)	-0.0047 (9)	-0.0085 (8)
C13A	0.0332 (11)	0.0363 (11)	0.0263 (10)	0.0013 (9)	-0.0014 (8)	-0.0092 (8)
C14A	0.0266 (10)	0.0301 (10)	0.0260 (10)	-0.0017 (8)	-0.0016 (8)	-0.0016 (8)
C15A	0.0254 (10)	0.0278 (10)	0.0240 (10)	-0.0017 (8)	-0.0029 (8)	-0.0019 (8)
O3B	0.0248 (7)	0.0375 (8)	0.0274 (7)	-0.0005 (6)	-0.0022 (5)	-0.0034 (6)
O4B	0.0282 (8)	0.0494 (9)	0.0217 (7)	0.0018 (6)	-0.0026 (6)	-0.0090 (6)
N4B	0.0276 (9)	0.0528 (11)	0.0283 (9)	-0.0019 (8)	-0.0064 (7)	-0.0134 (8)
C9B	0.0260 (10)	0.0242 (9)	0.0216 (9)	-0.0034 (8)	-0.0003 (7)	0.0004 (7)
C10B	0.0257 (10)	0.0244 (9)	0.0251 (10)	-0.0044 (8)	-0.0022 (8)	-0.0006 (7)
C11B	0.0323 (11)	0.0319 (10)	0.0241 (10)	-0.0029 (8)	-0.0014 (8)	-0.0069 (8)
C12B	0.0318 (11)	0.0295 (10)	0.0316 (11)	-0.0041 (9)	0.0054 (8)	-0.0070 (8)
C13B	0.0241 (10)	0.0343 (11)	0.0355 (11)	-0.0009 (8)	-0.0003 (8)	-0.0066 (9)
C14B	0.0267 (10)	0.0347 (11)	0.0287 (10)	-0.0010 (8)	-0.0045 (8)	-0.0049 (8)
C15B	0.0257 (10)	0.0293 (10)	0.0218 (9)	-0.0038 (8)	-0.0021 (8)	0.0002 (7)

Geometric parameters (Å, °)

O1A—C4A	1.340 (2)	C7A—H7A2	0.9598
O1A—C7A	1.437 (2)	C7A—H7A1	0.9599
O2A—C6A	1.344 (2)	C7A—H7A3	0.9598
O2A—C8A	1.428 (2)	C8A—H8A2	0.9604
O1B—C4B	1.342 (2)	C8A—H8A1	0.9595
O1B—C7B	1.433 (3)	C8A—H8A3	0.9594
O2B—C6B	1.342 (2)	C4B—C5B	1.387 (3)
O2B—C8B	1.426 (2)	C5B—C6B	1.367 (2)
O3A—C15A	1.315 (2)	C5B—H5B	0.9293
O4A—C15A	1.230 (2)	C7B—H7B1	0.9595
O3A—H3A	0.8200	C7B—H7B3	0.9599
O3B—C15B	1.232 (3)	C7B—H7B2	0.9600
O4B—C15B	1.310 (2)	C8B—H8B3	0.9605
O4B—H4B	0.8193	C8B—H8B2	0.9602
N1A—C2A	1.342 (2)	C8B—H8B1	0.9599
N1A—C6A	1.338 (2)	C9A—C15A	1.469 (2)
N2A—C2A	1.338 (2)	C9A—C10A	1.407 (2)
N3A—C4A	1.321 (2)	C9A—C14A	1.398 (3)
N3A—C2A	1.352 (2)	C10A—C11A	1.401 (3)
N2A—H2A2	0.8605	C11A—C12A	1.364 (3)
N2A—H2A1	0.8598	C12A—C13A	1.387 (3)
N1B—C6B	1.343 (2)	C13A—C14A	1.374 (3)
N1B—C2B	1.338 (3)	C11A—H11A	0.9303

N2B—C2B	1.333 (2)	C12A—H12A	0.9302
N3B—C4B	1.324 (2)	C13A—H13A	0.9300
N3B—C2B	1.351 (2)	C14A—H14A	0.9304
N2B—H2B1	0.8608	C9B—C15B	1.475 (3)
N2B—H2B2	0.8604	C9B—C10B	1.402 (3)
N4A—C10A	1.369 (2)	C9B—C14B	1.399 (3)
N4A—H7	0.91 (2)	C10B—C11B	1.406 (3)
N4A—H16	0.87 (2)	C11B—C12B	1.364 (3)
N4B—C10B	1.361 (3)	C12B—C13B	1.382 (3)
N4B—H4B2	0.8602	C13B—C14B	1.368 (3)
N4B—H4B1	0.8601	C11B—H11B	0.9304
C4A—C5A	1.387 (2)	C12B—H12B	0.9297
C5A—C6A	1.373 (2)	C13B—H13B	0.9295
C5A—H5A	0.9299	C14B—H14B	0.9302
O1B…C8A	3.366 (2)	C7B…H2B2 ^{viii}	2.9499
O2A…O3A	3.1345 (18)	C8A…H5A	2.5674
O2A…C11B ⁱ	3.386 (3)	C8B…H5B	2.5643
O2B…O4B	3.0386 (18)	C8B…H14B ⁱⁱⁱ	2.6313
O3A…O2A	3.1345 (18)	C10B…H5A ⁱⁱ	2.8828
O3A…N1A	2.6808 (19)	C11A…H7A1 ^{xv}	3.0702
O3B…C8B ⁱ	3.339 (2)	C11B…H5A ⁱⁱ	2.8311
O3B…N4B	2.749 (2)	C11B…H12A ^{xiii}	2.9790
O3B…N2B	3.075 (2)	C12A…H12B ^{xiii}	2.8221
O4A…N4A	2.650 (2)	C12B…H13A ^{xiii}	2.9326
O4A…N2A	2.818 (2)	C12B…H12A ^{xiii}	2.9020
O4B…C7B ⁱⁱ	3.405 (3)	C13A…H12B ^{xiii}	2.9162
O4B…O2B	3.0386 (18)	C13B…H4B1 ^{xiv}	3.0357
O4B…C6B ⁱ	3.320 (2)	C15A…H2A1	2.9083
O4B…C6B	3.348 (2)	C15A…H7	2.55 (2)
O4B…N1B	2.603 (2)	C15B…H4B1	2.6288
O1A…H11B ⁱⁱ	2.8584	C15B…H2B1	3.0282
O1B…H8A1	2.8768	H2A1…C7A ^{vi}	3.0537
O2A…H3A	2.6478	H2A1…C15A	2.9083
O2A…H11B ⁱ	2.8917	H2A1…H7A3 ^{vi}	2.4003
O2B…H4B	2.6746	H2A1…O4A	1.9706
O3A…H4B2 ⁱ	2.5912	H2A2…H7A3 ^{vi}	2.3895
O3A…H12B ⁱⁱⁱ	2.7485	H2A2…H2A2 ^{vi}	2.3863
O3A…H14A	2.4228	H2A2…C7A ^{vi}	3.0049
O3B…H8B3 ⁱ	2.4721	H2A2…H7 ^{vii}	2.3871
O3B…H2B1	2.2238	H2A2…N4A ^{vii}	2.8055
O3B…H4B1	2.1213	H2A2…N3A ^{vi}	2.3451
O4A…H7	1.97 (2)	H2A2…C2A ^{vi}	3.0643
O4A…H7A3 ^{iv}	2.7343	H7A1…C11A ^{xvi}	3.0702
O4A…H2A1	1.9706	H7A1…H11A ^{xvi}	2.3548
O4B…H7B2 ⁱⁱ	2.8459	H3A…C6A	2.7105
O4B…H14B	2.3016	H3A…C2A	2.8994
N1A…C15A	3.413 (2)	H3A…N1A	1.8629

N1A...O3A	2.6808 (19)	H3A...O2A	2.6478
N1B...O4B	2.603 (2)	H7A2...N3A	2.6166
N2A...C11A ^v	3.429 (3)	H7A2...N4A ^{xiii}	2.9272
N2A...O4A	2.818 (2)	H4B...C2B	2.8079
N2A...N3A ^{vi}	3.166 (2)	H4B...N1B	1.8054
N2A...N4A ^{vii}	3.223 (2)	H4B...C6B	2.6964
N2A...C7A ^{vi}	3.355 (3)	H4B...O2B	2.6746
N2B...O3B	3.075 (2)	H4B...H2B1	2.5495
N2B...C7B ^{viii}	3.324 (3)	H7A3...H2A2 ^{vi}	2.3895
N2B...N3B ^{viii}	3.165 (2)	H7A3...H2A1 ^{vi}	2.4003
N3A...N2A ^{vi}	3.166 (2)	H7A3...O4A ^v	2.7343
N3B...N2B ^{viii}	3.165 (2)	H7A3...N2A ^{vi}	2.7065
N4A...N4A ^{ix}	3.100 (3)	H7A3...N3A	2.6110
N4A...O4A	2.650 (2)	H5A...C11B ⁱⁱ	2.8311
N4A...N2A ^{vii}	3.223 (2)	H5A...H8A2	2.3603
N4B...C13B ^x	3.424 (3)	H5A...C10B ⁱⁱ	2.8828
N4B...O3B	2.749 (2)	H5A...N4B ⁱⁱ	2.9299
N1A...H3A	1.8629	H5A...C8A	2.5674
N1B...H4B	1.8054	H5A...H8A3	2.3629
N2A...H7 ^{vii}	2.72 (2)	H5B...H8B3	2.3881
N2A...H7A3 ^{vi}	2.7065	H5B...C8B	2.5643
N2B...H7B2 ^{viii}	2.7691	H5B...H8B2	2.3237
N3A...H16 ^{vii}	2.79 (2)	H8A1...O1B	2.8768
N3A...H7A3	2.6110	H7...H2A2 ^{vii}	2.3871
N3A...H2A2 ^{vi}	2.3450	H7...O4A	1.97 (2)
N3A...H7A2	2.6166	H7...N2A ^{vii}	2.72 (2)
N3B...H8B2 ^x	2.8142	H7...C15A	2.55 (2)
N3B...H7B3	2.6125	H8A2...C5A	2.7552
N3B...H7B2	2.6081	H8A2...H5A	2.3603
N3B...H2B2 ^{viii}	2.3290	H8A3...H5A	2.3629
N4A...H7A2 ^{xi}	2.9272	H8A3...N4B ⁱⁱ	2.8226
N4A...H16 ^{ix}	2.58 (2)	H8A3...C5A	2.7598
N4A...H11A ^{ix}	2.8681	H2B1...H4B	2.5495
N4A...H2A2 ^{vii}	2.8055	H2B1...C7B ^{viii}	3.0355
N4B...H5A ⁱⁱ	2.9299	H2B1...H7B2 ^{viii}	2.4952
N4B...H8A3 ⁱⁱ	2.8226	H2B1...C15B	3.0282
N4B...H13B ^x	2.7127	H2B1...O3B	2.2238
C2A...C10A ^v	3.331 (2)	H2B2...N3B ^{viii}	2.3290
C2A...C11A ^v	3.458 (3)	H2B2...C2B ^{viii}	3.0727
C2B...C5B ⁱⁱ	3.558 (2)	H2B2...C7B ^{viii}	2.9499
C2B...C6B ⁱⁱ	3.401 (2)	H2B2...H2B2 ^{viii}	2.4004
C4A...C9A ^v	3.539 (2)	H2B2...H7B2 ^{viii}	2.4198
C4A...C15A ^v	3.488 (3)	H8B1...H14B ⁱⁱⁱ	2.4098
C5A...C12A ^{xii}	3.537 (3)	H11A...H16	2.3411
C5A...C13A ^{xii}	3.447 (3)	H11A...H7A1 ^{xv}	2.3548
C5B...C15B ⁱ	3.341 (2)	H11A...N4A ^{ix}	2.8681
C5B...C2B ⁱⁱ	3.558 (2)	H11B...H4B2	2.3639
C5B...C9B ⁱ	3.559 (2)	H11B...H12A ^{xiii}	2.4408

C6A...C12A ^{xii}	3.493 (3)	H11B...O1A ⁱⁱ	2.8584
C6B...O4B	3.348 (2)	H11B...O2A ⁱ	2.8917
C6B...O4B ⁱ	3.320 (2)	H8B2...H5B	2.3237
C6B...C2B ⁱⁱ	3.401 (2)	H8B2...N3B ^{xiv}	2.8142
C6B...C15B ⁱ	3.514 (2)	H8B2...C5B	2.7274
C7A...N2A ^{vi}	3.355 (3)	H12A...C12B ^{xiii}	2.9019
C7B...O4B ⁱⁱ	3.405 (3)	H12A...C11B ^{xiii}	2.9790
C7B...N2B ^{viii}	3.324 (3)	H12A...H11B ^{xiii}	2.4408
C8A...O1B	3.366 (2)	H12A...H12B ^{xiii}	2.2849
C8B...O3B ⁱ	3.339 (2)	H12B...O3A ⁱⁱⁱ	2.7485
C8B...C14B ⁱⁱⁱ	3.447 (3)	H12B...C12A ^{xiii}	2.8220
C9A...C4A ^{iv}	3.539 (2)	H12B...C13A ^{xiii}	2.9162
C9B...C5B ⁱ	3.559 (2)	H12B...H12A ^{xiii}	2.2849
C10A...C2A ^{iv}	3.331 (2)	H12B...H13A ^{xiii}	2.4834
C11A...N2A ^{iv}	3.429 (3)	H8B3...H5B	2.3881
C11A...C2A ^{iv}	3.458 (3)	H8B3...O3B ⁱ	2.4721
C11B...O2A ⁱ	3.386 (3)	H8B3...C5B	2.7678
C12A...C5A ^{xi}	3.537 (3)	H8B3...H14B ⁱⁱⁱ	2.3522
C12A...C6A ^{xi}	3.493 (3)	H13A...H12B ^{xiii}	2.4834
C12A...C12B ^{xiii}	3.517 (3)	H13A...C12B ^{xiii}	2.9326
C12B...C13A ^{xiii}	3.526 (3)	H13B...N4B ^{xiv}	2.7127
C12B...C12A ^{xiii}	3.517 (3)	H13B...H4B1 ^{xiv}	2.3894
C13A...C5A ^{xi}	3.447 (3)	H14A...H4B2 ⁱ	2.5915
C13A...C12B ^{xiii}	3.526 (3)	H14A...O3A	2.4228
C13B...N4B ^{xiv}	3.424 (3)	H14B...C8B ⁱⁱⁱ	2.6313
C14B...C8B ⁱⁱⁱ	3.447 (3)	H14B...O4B	2.3016
C15A...N1A	3.413 (2)	H14B...H8B1 ⁱⁱⁱ	2.4098
C15A...C4A ^{iv}	3.488 (3)	H14B...H8B3 ⁱⁱⁱ	2.3522
C15B...C5B ⁱ	3.341 (2)	H7B2...N2B ^{viii}	2.7691
C15B...C6B ⁱ	3.514 (2)	H7B2...O4B ⁱⁱ	2.8459
C2A...H3A	2.8994	H7B2...H2B1 ^{viii}	2.4952
C2A...H2A2 ^{vi}	3.0643	H7B2...H2B2 ^{viii}	2.4198
C2B...H2B2 ^{viii}	3.0727	H7B2...N3B	2.6081
C2B...H4B	2.8079	H16...H16 ^{ix}	2.28 (3)
C5A...H8A3	2.7598	H16...H11A	2.3411
C5A...H8A2	2.7552	H16...N4A ^{ix}	2.58 (2)
C5B...H8B3	2.7678	H16...N3A ^{vii}	2.79 (2)
C5B...H8B2	2.7274	H7B3...N3B	2.6125
C6A...H3A	2.7105	H4B1...O3B	2.1213
C6B...H4B	2.6964	H4B1...C13B ^x	3.0357
C7A...H2A2 ^{vi}	3.0049	H4B1...C15B	2.6288
C7A...H2A1 ^{vi}	3.0537	H4B1...H13B ^x	2.3894
C7B...H2B1 ^{viii}	3.0355	H4B2...H11B	2.3639
C4A—O1A—C7A	118.05 (15)	C4B—C5B—H5B	122.42
C6A—O2A—C8A	118.02 (14)	C6B—C5B—H5B	122.43
C4B—O1B—C7B	117.81 (15)	O1B—C7B—H7B2	109.47
C6B—O2B—C8B	117.41 (15)	O1B—C7B—H7B3	109.50

C15A—O3A—H3A	109.45	O1B—C7B—H7B1	109.50
C15B—O4B—H4B	109.42	H7B2—C7B—H7B3	109.50
C2A—N1A—C6A	116.21 (14)	H7B1—C7B—H7B2	109.40
C2A—N3A—C4A	114.84 (15)	H7B1—C7B—H7B3	109.45
C2A—N2A—H2A1	120.01	H8B1—C8B—H8B2	109.51
C2A—N2A—H2A2	120.03	O2B—C8B—H8B3	109.49
H2A1—N2A—H2A2	119.95	O2B—C8B—H8B2	109.50
C2B—N1B—C6B	116.94 (16)	O2B—C8B—H8B1	109.46
C2B—N3B—C4B	114.73 (16)	H8B1—C8B—H8B3	109.45
H2B1—N2B—H2B2	119.91	H8B2—C8B—H8B3	109.41
C2B—N2B—H2B1	120.04	C10A—C9A—C15A	120.50 (15)
C2B—N2B—H2B2	120.05	C14A—C9A—C15A	120.32 (16)
H7—N4A—H16	118 (2)	C10A—C9A—C14A	119.16 (15)
C10A—N4A—H7	116.0 (15)	N4A—C10A—C11A	118.55 (16)
C10A—N4A—H16	116.8 (15)	C9A—C10A—C11A	118.15 (16)
C10B—N4B—H4B1	120.00	N4A—C10A—C9A	123.30 (15)
C10B—N4B—H4B2	120.00	C10A—C11A—C12A	121.29 (19)
H4B1—N4B—H4B2	120.01	C11A—C12A—C13A	121.0 (2)
N1A—C2A—N2A	116.23 (14)	C12A—C13A—C14A	118.69 (19)
N1A—C2A—N3A	125.95 (16)	C9A—C14A—C13A	121.71 (18)
N2A—C2A—N3A	117.82 (16)	O4A—C15A—C9A	122.52 (16)
N3A—C4A—C5A	124.69 (14)	O3A—C15A—C9A	115.63 (15)
O1A—C4A—N3A	119.51 (15)	O3A—C15A—O4A	121.84 (15)
O1A—C4A—C5A	115.79 (15)	C10A—C11A—H11A	119.34
C4A—C5A—C6A	115.23 (16)	C12A—C11A—H11A	119.36
O2A—C6A—C5A	125.55 (16)	C13A—C12A—H12A	119.48
O2A—C6A—N1A	111.41 (14)	C11A—C12A—H12A	119.53
N1A—C6A—C5A	123.04 (16)	C12A—C13A—H13A	120.66
C6A—C5A—H5A	122.42	C14A—C13A—H13A	120.65
C4A—C5A—H5A	122.35	C9A—C14A—H14A	119.12
O1A—C7A—H7A2	109.37	C13A—C14A—H14A	119.18
H7A1—C7A—H7A3	109.49	C14B—C9B—C15B	118.51 (17)
O1A—C7A—H7A3	109.51	C10B—C9B—C14B	118.82 (17)
H7A1—C7A—H7A2	109.42	C10B—C9B—C15B	122.68 (19)
O1A—C7A—H7A1	109.53	N4B—C10B—C11B	119.07 (17)
H7A2—C7A—H7A3	109.50	C9B—C10B—C11B	118.18 (19)
H8A2—C8A—H8A3	109.48	N4B—C10B—C9B	122.75 (17)
H8A1—C8A—H8A3	109.47	C10B—C11B—C12B	121.16 (18)
O2A—C8A—H8A3	109.55	C11B—C12B—C13B	121.0 (2)
H8A1—C8A—H8A2	109.44	C12B—C13B—C14B	118.7 (2)
O2A—C8A—H8A2	109.46	C9B—C14B—C13B	122.10 (18)
O2A—C8A—H8A1	109.42	O3B—C15B—C9B	124.16 (17)
N2B—C2B—N3B	118.31 (18)	O4B—C15B—C9B	112.92 (18)
N1B—C2B—N2B	116.21 (16)	O3B—C15B—O4B	122.92 (16)
N1B—C2B—N3B	125.48 (17)	C10B—C11B—H11B	119.44
N3B—C4B—C5B	125.03 (16)	C12B—C11B—H11B	119.40
O1B—C4B—N3B	119.61 (17)	C11B—C12B—H12B	119.59
O1B—C4B—C5B	115.36 (17)	C13B—C12B—H12B	119.46

C4B—C5B—C6B	115.15 (18)	C12B—C13B—H13B	120.60
O2B—C6B—N1B	111.18 (15)	C14B—C13B—H13B	120.71
O2B—C6B—C5B	126.17 (18)	C9B—C14B—H14B	118.94
N1B—C6B—C5B	122.65 (19)	C13B—C14B—H14B	118.95
C7A—O1A—C4A—N3A	1.2 (2)	C4B—C5B—C6B—O2B	179.87 (16)
C7A—O1A—C4A—C5A	-179.01 (17)	C14A—C9A—C15A—O4A	174.43 (19)
C8A—O2A—C6A—N1A	179.08 (17)	C15A—C9A—C10A—N4A	2.6 (2)
C8A—O2A—C6A—C5A	-1.1 (3)	C15A—C9A—C10A—C11A	-178.15 (17)
C7B—O1B—C4B—N3B	0.6 (2)	C14A—C9A—C10A—N4A	-178.92 (17)
C7B—O1B—C4B—C5B	-179.14 (16)	C14A—C9A—C10A—C11A	0.3 (2)
C8B—O2B—C6B—C5B	-1.5 (3)	C10A—C9A—C14A—C13A	-0.5 (3)
C8B—O2B—C6B—N1B	178.82 (15)	C15A—C9A—C14A—C13A	177.98 (19)
C2A—N1A—C6A—O2A	-179.97 (17)	C10A—C9A—C15A—O4A	-7.1 (3)
C6A—N1A—C2A—N3A	-1.4 (2)	C14A—C9A—C15A—O3A	-6.4 (3)
C6A—N1A—C2A—N2A	178.93 (16)	C10A—C9A—C15A—O3A	172.05 (16)
C2A—N1A—C6A—C5A	0.2 (3)	C9A—C10A—C11A—C12A	-0.5 (3)
C4A—N3A—C2A—N1A	1.1 (2)	N4A—C10A—C11A—C12A	178.82 (19)
C4A—N3A—C2A—N2A	-179.32 (14)	C10A—C11A—C12A—C13A	0.8 (3)
C2A—N3A—C4A—O1A	-179.60 (14)	C11A—C12A—C13A—C14A	-0.9 (3)
C2A—N3A—C4A—C5A	0.6 (2)	C12A—C13A—C14A—C9A	0.8 (3)
C6B—N1B—C2B—N3B	-1.7 (3)	C10B—C9B—C15B—O3B	4.9 (3)
C2B—N1B—C6B—C5B	1.0 (2)	C10B—C9B—C15B—O4B	-175.17 (15)
C2B—N1B—C6B—O2B	-179.28 (14)	C14B—C9B—C15B—O3B	-175.29 (17)
C6B—N1B—C2B—N2B	179.12 (15)	C14B—C9B—C15B—O4B	4.7 (2)
C4B—N3B—C2B—N2B	-179.14 (15)	C15B—C9B—C10B—N4B	3.4 (2)
C4B—N3B—C2B—N1B	1.7 (2)	C15B—C9B—C10B—C11B	-176.60 (16)
C2B—N3B—C4B—C5B	-1.0 (2)	C10B—C9B—C14B—C13B	-2.2 (3)
C2B—N3B—C4B—O1B	179.26 (15)	C15B—C9B—C14B—C13B	177.97 (18)
O1A—C4A—C5A—C6A	178.51 (17)	C14B—C9B—C10B—N4B	-176.38 (17)
N3A—C4A—C5A—C6A	-1.7 (3)	C14B—C9B—C10B—C11B	3.6 (2)
C4A—C5A—C6A—N1A	1.3 (3)	N4B—C10B—C11B—C12B	177.68 (18)
C4A—C5A—C6A—O2A	-178.56 (18)	C9B—C10B—C11B—C12B	-2.3 (3)
N3B—C4B—C5B—C6B	0.5 (3)	C10B—C11B—C12B—C13B	-0.6 (3)
O1B—C4B—C5B—C6B	-179.79 (15)	C11B—C12B—C13B—C14B	2.0 (3)
C4B—C5B—C6B—N1B	-0.4 (2)	C12B—C13B—C14B—C9B	-0.6 (3)

Symmetry codes: (i) $-x+2, -y+2, -z+1$; (ii) $-x+2, -y+1, -z+1$; (iii) $-x+1, -y+2, -z+1$; (iv) $x, y+1, z$; (v) $x, y-1, z$; (vi) $-x+2, -y+1, -z$; (vii) $-x+2, -y+2, -z$; (viii) $-x+3, -y+1, -z+1$; (ix) $-x+1, -y+3, -z$; (x) $x+1, y, z$; (xi) $x-1, y+1, z$; (xii) $x+1, y-1, z$; (xiii) $-x+1, -y+3, -z+1$; (xiv) $x-1, y, z$; (xv) $x-1, y+2, z$; (xvi) $x+1, y-2, z$.

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N2A—H2A1 \cdots O4A	0.86	1.97	2.818 (2)	169
N2A—H2A2 \cdots N3A ^{vi}	0.86	2.35	3.166 (2)	160
O3A—H3A \cdots N1A	0.82	1.86	2.6808 (19)	175
O4B—H4B \cdots N1B	0.82	1.81	2.603 (2)	164
N4A—H7 \cdots O4A	0.91 (2)	1.97 (2)	2.650 (2)	130 (2)

N2B—H2B1···O3B	0.86	2.22	3.075 (2)	170
N2B—H2B2···N3B ^{viii}	0.86	2.33	3.165 (2)	164
N4A—H16···N4A ^{ix}	0.87 (2)	2.58 (2)	3.100 (3)	119.7 (18)
N4B—H4B1···O3B	0.86	2.12	2.749 (2)	129
N4B—H4B2···O3A ⁱ	0.86	2.59	3.450 (2)	176
C8B—H8B3···O3B ⁱ	0.96	2.47	3.339 (2)	150
C14A—H14A···O3A	0.93	2.42	2.747 (3)	100
C14B—H14B···O4B	0.93	2.30	2.655 (2)	102

Symmetry codes: (i) $-x+2, -y+2, -z+1$; (vi) $-x+2, -y+1, -z$; (viii) $-x+3, -y+1, -z+1$; (ix) $-x+1, -y+3, -z$.