IUCrData

ISSN 2414-3146

N-(4-Amino-1,2,5-oxadiazol-3-yl)formamide

Firudin I. Guseinov,[a,b] Tuncer Hökelek,[c] Elena V. Shuvalova,[b] Aida I. Samigullina,[b] Nizami A. Ekberov,[d] Khudayar I. Hasanov[e] and Mohammed Hadi Al-Douh[f]*

[a]Kosygin State University of Russia, 117997 Moscow, Russian Federation, [b]N. D. Zelinsky Institute of Organic Chemistry, Russian Academy of Sciences, 119991 Moscow, Russian Federation, [c]Hacettepe University, Department of Physics, 06800 Beytepe-Ankara, Türkiye, [d]Azerbaijan State Pedagogical University, 68 Uzeyir Hajibeyov St., AZ 1000, Baku, Azerbaijan, [e]Azerbaijan Medical University, Scientific Research Centre (SRC), A. Kasumzade St. 14, AZ1022 Baku, Azerbaijan, and [f]Chemistry Department, Faculty of Science, Hadhramout University, Mukalla, Hadhramout, Yemen. *Correspondence e-mail: m.aldouh@hu.edu.ye

Received 25 June 2025
Accepted 13 August 2025

Edited by M. Weil, Vienna University of Technology, Austria

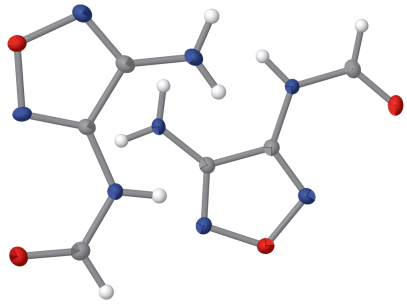
Keywords: crystal structure; non-covalent interactions; 2,2-dihalo-3-oxoaldehydes; pyrazol.

CCDC reference: 2480423

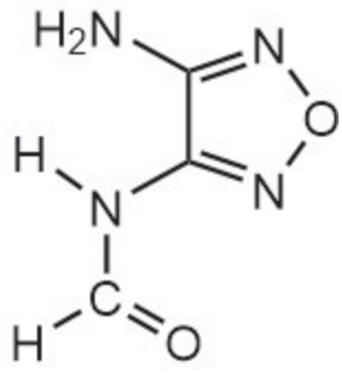
Structural data: full structural data are available from iucrdata.iucr.org

The asymmetric unit of the title compound, $C_3H_4N_4O_2$, contains two coplanar molecules (*A* and *B*) completely located on mirror planes. In the crystal, N—H···O, N—H···N, C—H···O and C—H···N hydrogen bonds link the molecules into sheets parallel to (010). There are neither significant π–π nor C—H···π(ring) interactions. Hirshfeld surface analysis indicates that the most important contributions to the crystal packings of molecules *A* and *B* are from H···O/O···H (32.4% for *A*, 30.1% for *B*), H···N/N···H (28.2%, 31.5%) and H···H (12.3%, 8.0%) interactions.

3D view



Chemical scheme



Structure description

Oxadiazole is a five-membered heterocyclic compound with one oxygen and two nitrogen atoms. The oxadiazole scaffold is a commonly utilized pharmacophore and has been subjected to extensive studies in recent years because of its metabolic profile and ability to engage in hydrogen-bonding with receptor sites (Khan *et al.*, 2017; Khalilov, 2021). Oxadiazole derivatives have also attracted significant attention because of their reactivity (Guseinov *et al.*, 2024), diverse functional (Aliyeva *et al.*, 2024) and pharmacological properties, including anti-inflammatory, antibacterial, antihypertension, muscle relaxing and anticancer activities (Boström *et al.*, 2012). Moreover, derivatization of the oxadiazole synthon with non-covalent donor or acceptor sites for hydrogen-bonding interactions can be applied as a synthetic strategy in the improvement of functional properties of its metal complexes (Mahmudov *et al.*, 2022). Herein, we report synthesis, molecular and crystal structures together with Hirshfeld surface analysis of a new aldehyde and NH-functionalized oxadiazole derivative, $C_3H_4N_4O_2$.

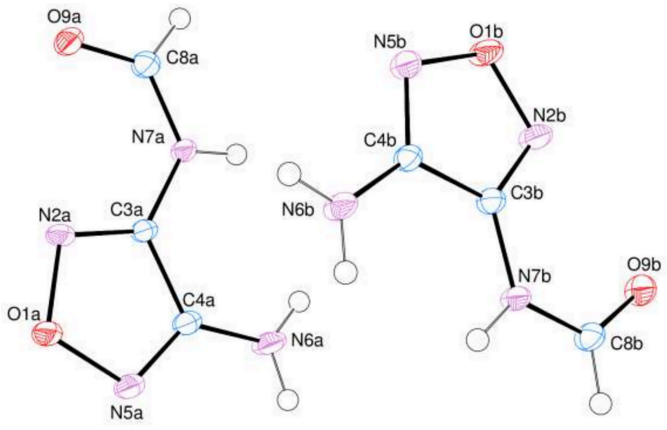


Figure 1
The asymmetric unit of the title compound with the atom-numbering scheme and 50% probability ellipsoids.

The asymmetric unit contains two molecules (*A* and *B*, Fig. 1) completely located on mirror planes, making the molecules exactly planar. Small variations are observed in the C8*A*—N7*A*—C3*A* [125.88 (14)°] and C8*B*—N7*B*—C3*B* [125.04 (14)°], N2*A*—C3*A*—N7*A* [125.07 (14)°] and N2*B*—C3*B*—N7*B* [125.41 (14)°], N7*A*—C3*A*—C4*A* [124.71 (14)°] and N7*B*—C3*B*—C4*B* [124.10 (14)°], N5*A*—C4*A*—N6*A* [124.68 (15)°] and N5*B*—C4*B*—N6*B* [125.28 (15)°], N6*A*—C4*A*—C3*A* [127.25 (15)°] and N6*B*—C4*B*—C3*B* [126.16 (15)°], O9*A*—C8*A*—N7*A* [125.23 (15)°] and O9B—C8B—N7B [123.42 (15)°] bond angles due to the strengths of the N—H···O and N—H···N hydrogen-bonding interactions (Fig. 2,Table 1). Next to these classical hydrogen-bonding interactions, weaker C—H···O and C—H···N interactions are also present (Table 1), linking the molecules into sheets extending parallel to (010). There are neither significant π–π nor C—H···π(ring) interactions present between molecules.

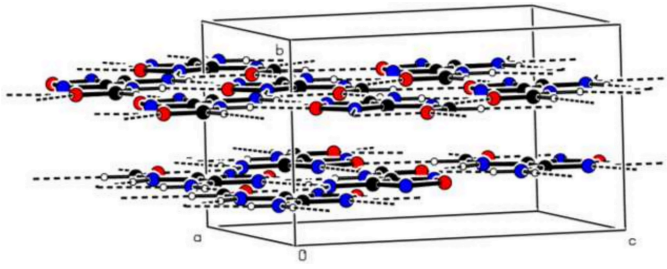


Figure 2
Partial packing diagram of the title compound, highlighting the layered arrangement. Intermolecular N—H···N, N—H···O, C—H···O and C—H···N hydrogen bonds are shown as dashed lines.

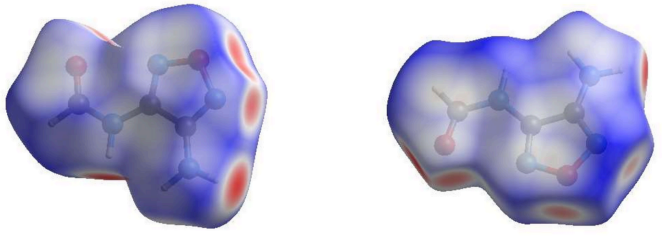


Figure 3
Views of the three-dimensional Hirshfeld surfaces for (*a*) molecule *A* and (*b*) molecule *B* plotted over d_{norm}.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N6*A*—H6*A*···O9*A*^{i}	0.88 (3)	2.05 (3)	2.9207 (19)	172 (2)
N6*A*—H6*B*···O9*B*^{ii}	0.83 (3)	2.26 (3)	3.074 (2)	164 (2)
N7*A*—H7*A*···O9*B*^{iii}	0.87 (3)	1.93 (3)	2.8033 (18)	177 (2)
N7*A*—H7*A*···O9*B*^{ii}	0.87 (3)	1.93 (3)	2.8033 (18)	177 (2)
N6*B*—H6*C*···N5*A*^{iv}	0.88 (2)	2.31 (2)	3.189 (2)	175 (2)
N6*B*—H6*D*···O9*A*^{v}	0.85 (3)	2.31 (3)	2.8121 (19)	118 (2)
N6*B*—H6*D*···N2*A*^{v}	0.85 (3)	2.20 (3)	3.0387 (19)	166 (3)
N7*B*—H7*B*···O1*A*^{iv}	0.91 (3)	2.24 (3)	3.0354 (17)	145 (2)
N7*B*—H7*B*···N5*A*^{iv}	0.91 (3)	2.32 (3)	3.2302 (19)	179 (2)
C8*A*—H8*A*···O1*B*^{vi}	0.95	2.32	3.266 (2)	175
C8*B*—H8*B*···N5*B*^{vii}	0.95	2.55	3.489 (2)	170

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

Table 2
Comparison of the percentage contributions to the crystal packing for molecules *A* and *B*.

Contacts	*A*	*B*
H···O/O···H	32.4	30.1
H···N/N···H	28.2	31.5
H···H	12.3	8.0
H···C/C···H	7.2	6.9
N···O/O···N	5.3	4.3
O···O	4.6	1.5
C···O/O···C	3.9	7.2
C···N/N···C	3.3	5.6
N···N	2.9	5.0

A Hirshfeld surface (HS) analysis was carried out using *CrystalExplorer* (Spackman *et al.*, 2021) to visualize and quantify the intermolecular interactions. In the HSs plotted over d_{norm} (Fig. 3*a,b*), the contact distances equal, shorter and longer with respect to the sum of van der Waals radii are shown by white, red and blue colours, respectively. According to the two-dimensional fingerprint plots, H···O/O···H, H···N/N···H and H···H contacts make the most important contributions to the HSs (Table 2, Figs. 4 and 5), and they have significant differences due to the different numbers and values of the close contacts.

Synthesis and crystallization

A mixture of diaminofurazan (20 mg, 0.2 mmol) and 2,2-dichloro-3-oxo-3-phenylpropanal (42.4 mg, 0.2 mmol) in 15 ml of CCl_4 (dry) was boiled for 30 min. The reaction mixture was then cooled to room temperature, the precipitate filtered and recrystallized from chloroform solution. Yield 15.4 mg (62%), ^{1}H NMR (300 MHz, DMSO-d_6): 10.40 (1*H*, NH), 8.75 (1*H*, CHO), 6.11 (2*H*, NH_2). ^{13}C NMR (200 MHz, DMSO-d_6): 143.89, 147.78, 165.90.

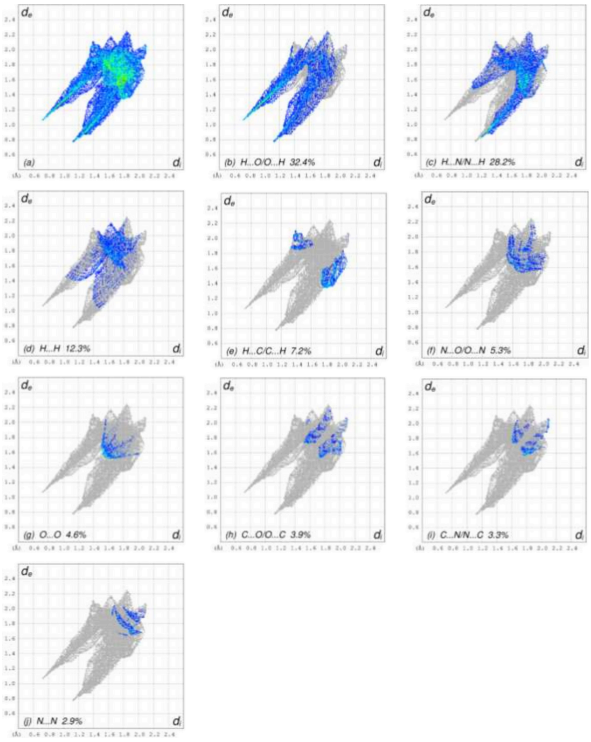


Figure 4
The full two-dimensional fingerprint plots for molecule *A*, showing (*a*) all interactions, and delineated into (*b*) H···O/O···H, (*c*) H···N/N···H, (*d*) H···H, (*e*) H···C/C···H, (*f*) N···O/O···N, (*g*) O···O, (*h*) C···O/O···C, (i) C···N/N···C and (*j*) N···N interactions. The d_i and d_e values are the closest internal and external distances (in Å) from given points on the Hirshfeld surface contacts.

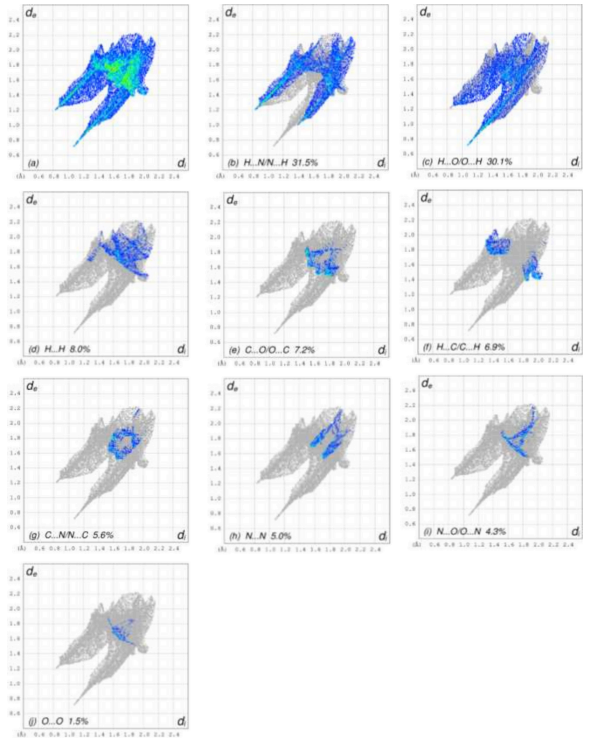


Figure 5
The full two-dimensional fingerprint plots for molecule *B*; subdivisions are the same as in Fig. 4.

Table 3
Experimental details.

Crystal data	
Chemical formula	$C_3H_4N_4O_2$
M_r	128.10
Crystal system, space group	Monoclinic, $P12_1/m1$
Temperature (K)	100
a, b, c (Å)	7.98085 (8), 6.17409 (7), 10.19204 (9)
β (°)	95.2595 (9)
V (Å^3)	500.09 (1)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	1.26
Crystal size (mm)	0.28 × 0.22 × 0.04
Data collection	
Diffractometer	XtaLAB Synergy, Dualflex, HyPix
Absorption correction	Gaussian (*CrysAlis PRO*; Rigaku OD, 2023)
T_{min}, T_{max}	0.503, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	13311, 1182, 1153
R_{int}	0.031
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.638
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.035, 0.095, 1.06
No. of reflections	1182
No. of parameters	128
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.45, −0.26

Computer programs: *CrysAlis PRO* (Rigaku OD, 2023), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*), *OLEX2* (Dolomanov *et al.*, 2009) and *publCIF* (Westrip, 2010).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3.

Acknowledgements

The crystal-structure determination was performed in the Department of Structural Studies of the Zelinsky Institute of Organic Chemistry, Moscow. This work has been supported by the Azerbaijan State Pedagogical University and Azerbaijan Medical University. The author's contributions are as follows. Conceptualization, FIG and ANB; synthesis, EVS; X-ray analysis, AIS and TH; Hirshfeld surface analysis, TH; writing (review and editing of the manuscript), TH, NAE and KIH; funding acquisition, NAE and KIH; supervision, FIG, TH and ANB.

References

Aliyeva, V. A., Gurbanov, A. V., Huseynov, F. E., Hajiyeva, S. R., Conceição, N. R., Nunes, A. V. M., Pombeiro, A. J. L. & Mahmudov, K. T. (2024). *Polyhedron* **255**, 116955.

Boström, J., Hogner, A., Llinàs, A., Wellner, E. & Plowright, A. T. (2012). *J. Med. Chem.* **55**, 1817–1830.

Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.

Guseinov, F. I., Ovsyannikov, V. O., Shuvalova, E. V., Kustov, L. M., Kobrakov, K. I., Samigullina, A. I. & Mahmudov, K. T. (2024). *New J. Chem.* **48**, 12869–12872.
Khalilov, A. N. (2021). *Rev. Roum. Chim.* **66**, 719.
Khan, I., Tantray, M. A., Alam, M. S. & Hamid, H. (2017). *Eur. J. Med. Chem.* **125**, 464–477.
Mahmudov, K. T., Kerimli, F. Sh., Mammadov, E. S., Gurbanov, A. V., Akhmedova, N. F. & Mammadov, S. E. (2022). *Pet. Chem.* **62**, 933–941.
Rigaku OD (2023). *CrysAlis PRO*. Oxford Diffraction, Yarnton, England.
Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.
Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.
Spackman, P. R., Turner, M. J., McKinnon, J. J., Wolff, S. K., Grimwood, D. J., Jayatilaka, D. & Spackman, M. A. (2021). *J. Appl. Cryst.* **54**, 1006–1011.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

full crystallographic data

IUCrData (2025). **10**, x250720 [https://doi.org/10.1107/S2414314625007205]

N-(4-Amino-1,2,5-oxadiazol-3-yl)formamide

Firudin I. Guseinov, Tuncer Hökelek, Elena V. Shuvalova, Aida I. Samigullina, Nizami A. Ekberov, Khudayar I. Hasanov and Mohammed Hadi Al-Douh

_N_-(4-Amino-1,2,5-oxadiazol-3-yl)formamide

Crystal data

$C_3H_4N_4O_2$
M_r = 128.10
Monoclinic, $P12_1/m1$
a = 7.98085 (8) Å
b = 6.17409 (7) Å
c = 10.19204 (9) Å
β = 95.2595 (9)°
V = 500.09 (1) Å^3
Z = 4
$F(000)$ = 264
D_x = 1.701 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54184 Å
Cell parameters from 9316 reflections
θ = 4.4–78.3°
μ = 1.26 mm^{-1}
T = 100 K
Prism, colorless
0.28 × 0.22 × 0.04 mm

Data collection

XtaLAB Synergy, Dualflex, HyPix diffractometer
Radiation source: micro-focus sealed X-ray tube, PhotonJet (Cu) X-ray Source
Mirror monochromator
Detector resolution: 10.0000 pixels mm^{-1}
ω scans
Absorption correction: gaussian (CrysAlisPro; Rigaku OD, 2023)
T_{min} = 0.503, T_{max} = 1.000
13311 measured reflections
1182 independent reflections
1153 reflections with $I > 2\sigma(I)$
R_{int} = 0.031
θ_{max} = 79.7°, θ_{min} = 4.4°
h = −10→10
k = −7→7
l = −12→12

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.095
S = 1.06
1182 reflections
128 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0568P)^2 + 0.2125P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 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: 0.0043 (10)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. The NH hydrogen atomss were located in difference-Fourier maps and were refined isotropically.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1A	0.21691 (14)	0.750000	−0.13259 (11)	0.0213 (3)
O9A	−0.19240 (15)	0.750000	0.09542 (12)	0.0223 (3)
N2A	0.08834 (16)	0.750000	−0.04954 (13)	0.0183 (3)
N5A	0.37506 (17)	0.750000	−0.05892 (14)	0.0212 (3)
N6A	0.46198 (18)	0.750000	0.16804 (16)	0.0309 (4)
H6A	0.569 (4)	0.750000	0.154 (3)	0.034 (6)*
H6B	0.433 (3)	0.750000	0.245 (3)	0.029 (6)*
N7A	0.08165 (16)	0.750000	0.18320 (13)	0.0181 (3)
H7A	0.141 (3)	0.750000	0.259 (3)	0.027 (6)*
C3A	0.16276 (19)	0.750000	0.06877 (15)	0.0163 (3)
C4A	0.34342 (19)	0.750000	0.06452 (16)	0.0191 (3)
C8A	−0.0871 (2)	0.750000	0.18991 (16)	0.0205 (4)
H8A	−0.126486	0.750000	0.275080	0.025*
O1B	0.19712 (15)	0.250000	0.50920 (12)	0.0247 (3)
O9B	0.71609 (15)	0.250000	0.57695 (12)	0.0226 (3)
N2B	0.37256 (17)	0.250000	0.52444 (14)	0.0230 (3)
N5B	0.13570 (18)	0.250000	0.37538 (14)	0.0213 (3)
N6B	0.26997 (19)	0.250000	0.17935 (14)	0.0259 (4)
H6C	0.365 (3)	0.250000	0.141 (2)	0.023 (5)*
H6D	0.177 (4)	0.250000	0.130 (3)	0.039 (7)*
N7B	0.58111 (16)	0.250000	0.37086 (13)	0.0187 (3)
H7B	0.595 (3)	0.250000	0.283 (3)	0.028 (6)*
C3B	0.4166 (2)	0.250000	0.40507 (15)	0.0176 (3)
C4B	0.26997 (19)	0.250000	0.31096 (16)	0.0170 (3)
C8B	0.7209 (2)	0.250000	0.45783 (16)	0.0201 (4)
H8B	0.827870	0.250000	0.423922	0.024*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1A	0.0133 (5)	0.0377 (7)	0.0134 (5)	0.000	0.0029 (4)	0.000
O9A	0.0136 (5)	0.0363 (7)	0.0165 (6)	0.000	0.0000 (4)	0.000
N2A	0.0123 (6)	0.0303 (7)	0.0130 (6)	0.000	0.0045 (5)	0.000
N5A	0.0117 (6)	0.0342 (8)	0.0178 (7)	0.000	0.0018 (5)	0.000
N6A	0.0101 (7)	0.0663 (12)	0.0164 (7)	0.000	0.0013 (5)	0.000
N7A	0.0109 (6)	0.0326 (8)	0.0106 (6)	0.000	0.0005 (5)	0.000
C3A	0.0107 (7)	0.0246 (8)	0.0136 (7)	0.000	0.0017 (5)	0.000
C4A	0.0117 (7)	0.0286 (8)	0.0170 (8)	0.000	0.0019 (6)	0.000

C8A	0.0159 (7)	0.0315 (9)	0.0145 (7)	0.000	0.0025 (6)	0.000
O1B	0.0137 (6)	0.0467 (8)	0.0141 (6)	0.000	0.0026 (4)	0.000
O9B	0.0177 (6)	0.0349 (7)	0.0143 (6)	0.000	−0.0027 (4)	0.000
N2B	0.0126 (6)	0.0404 (9)	0.0159 (7)	0.000	0.0017 (5)	0.000
N5B	0.0150 (6)	0.0361 (8)	0.0127 (6)	0.000	0.0006 (5)	0.000
N6B	0.0116 (7)	0.0540 (10)	0.0117 (6)	0.000	−0.0012 (5)	0.000
N7B	0.0113 (6)	0.0338 (8)	0.0109 (7)	0.000	0.0005 (5)	0.000
C3B	0.0136 (7)	0.0257 (8)	0.0133 (7)	0.000	0.0008 (6)	0.000
C4B	0.0128 (7)	0.0238 (8)	0.0142 (7)	0.000	0.0004 (5)	0.000
C8B	0.0137 (7)	0.0294 (9)	0.0169 (8)	0.000	−0.0010 (6)	0.000

Geometric parameters (Å, º)

O1A—N2A	1.3888 (16)	O1B—N2B	1.3945 (17)
O1A—N5A	1.4082 (17)	O1B—N5B	1.4064 (17)
O9A—C8A	1.219 (2)	O9B—C8B	1.218 (2)
N2A—C3A	1.294 (2)	N2B—C3B	1.297 (2)
N5A—C4A	1.306 (2)	N5B—C4B	1.307 (2)
N6A—H6A	0.88 (3)	N6B—H6C	0.88 (2)
N6A—H6B	0.83 (3)	N6B—H6D	0.85 (3)
N6A—C4A	1.351 (2)	N6B—C4B	1.341 (2)
N7A—H7A	0.87 (3)	N7B—H7B	0.91 (3)
N7A—C3A	1.385 (2)	N7B—C3B	1.389 (2)
N7A—C8A	1.355 (2)	N7B—C8B	1.360 (2)
C3A—C4A	1.446 (2)	C3B—C4B	1.444 (2)
C8A—H8A	0.9500	C8B—H8B	0.9500
O1A···N7B^{i}	3.0352 (18)	H6B···O9B^{ii}	2.26 (3)
O1B···C8B^{ii}	3.1671 (5)	N2A···N6B^{x}	3.039 (2)
O9A···N6B^{iii}	2.812 (2)	N2B···C8B^{v}	3.1849 (5)
O9A···N2A	2.7947 (18)	N6A···N7A	3.054 (2)
N6A···O9A^{iv}	2.9206 (19)	N6B···N7B	3.014 (2)
O9B···N7A^{v}	2.8032 (18)	N2A···H6D^{iii}	2.20 (3)
O9B···N6A^{vi}	3.074 (2)	H6B···N2B^{ii}	2.69 (3)
O9B···N2B	2.7448 (19)	N5A···H7B^{vii}	2.32 (3)
O1A···H7B^{vii}	2.24 (3)	N5A···H6C^{vii}	2.31 (2)
O1B···H8A^{viii}	2.3189	H8B···N5B^{xi}	2.55
H6D···O9A^{ix}	2.31 (3)	N6B···H7B	2.72 (3)
O9A···H6C^{iii}	2.66 (2)	C8A···H6A^{xii}	2.74 (3)
H6A···O9A^{iv}	2.06 (3)	H6B···H7A	2.35 (3)
H6D···O9A^{iii}	2.31 (3)	H6C···H7B	2.24 (4)
O9B···H7A^{vi}	1.94 (3)		
N2A—O1A—N5A	110.56 (11)	N2B—O1B—N5B	111.41 (11)
C3A—N2A—O1A	105.44 (12)	C3B—N2B—O1B	104.56 (13)
C4A—N5A—O1A	105.71 (12)	C4B—N5B—O1B	104.97 (13)
H6A—N6A—H6B	120 (2)	H6C—N6B—H6D	118 (2)
C4A—N6A—H6A	119.8 (17)	C4B—N6B—H6C	121.3 (15)

C4A—N6A—H6B	119.8 (17)	C4B—N6B—H6D	120.5 (18)
C3A—N7A—H7A	119.6 (16)	C3B—N7B—H7B	116.9 (15)
C8A—N7A—H7A	114.5 (16)	C8B—N7B—H7B	118.0 (15)
C8A—N7A—C3A	125.88 (14)	C8B—N7B—C3B	125.04 (14)
N2A—C3A—N7A	125.07 (14)	N2B—C3B—N7B	125.41 (14)
N2A—C3A—C4A	110.23 (13)	N2B—C3B—C4B	110.49 (14)
N7A—C3A—C4A	124.71 (14)	N7B—C3B—C4B	124.10 (14)
N5A—C4A—N6A	124.68 (15)	N5B—C4B—N6B	125.28 (15)
N5A—C4A—C3A	108.07 (14)	N5B—C4B—C3B	108.56 (14)
N6A—C4A—C3A	127.25 (15)	N6B—C4B—C3B	126.16 (15)
O9A—C8A—N7A	125.23 (15)	O9B—C8B—N7B	123.42 (15)
O9A—C8A—H8A	117.4	O9B—C8B—H8B	118.3
N7A—C8A—H8A	117.4	N7B—C8B—H8B	118.3
O1A—N2A—C3A—N7A	180.000 (1)	O1B—N2B—C3B—N7B	180.000 (1)
O1A—N2A—C3A—C4A	0.0	O1B—N2B—C3B—C4B	0.000 (1)
O1A—N5A—C4A—N6A	180.000 (1)	O1B—N5B—C4B—N6B	180.000 (1)
O1A—N5A—C4A—C3A	0.0	O1B—N5B—C4B—C3B	0.000 (1)
N2A—O1A—N5A—C4A	0.000 (1)	N2B—O1B—N5B—C4B	0.000 (1)
N2A—C3A—C4A—N5A	0.0	N2B—C3B—C4B—N5B	0.000 (1)
N2A—C3A—C4A—N6A	180.000 (1)	N2B—C3B—C4B—N6B	180.000 (1)
N5A—O1A—N2A—C3A	0.000 (1)	N5B—O1B—N2B—C3B	0.000 (1)
N7A—C3A—C4A—N5A	180.0	N7B—C3B—C4B—N5B	180.000 (1)
N7A—C3A—C4A—N6A	0.000 (1)	N7B—C3B—C4B—N6B	0.000 (1)
C3A—N7A—C8A—O9A	0.000 (1)	C3B—N7B—C8B—O9B	0.000 (1)
C8A—N7A—C3A—N2A	0.000 (1)	C8B—N7B—C3B—N2B	0.000 (1)
C8A—N7A—C3A—C4A	180.000 (1)	C8B—N7B—C3B—C4B	180.000 (1)

Symmetry codes: (i) −*x*+1, *y*+1/2, −*z*; (ii) −*x*+1, *y*+1/2, −*z*+1; (iii) −*x*, −*y*+1, −*z*; (iv) *x*+1, *y*, *z*; (v) −*x*+1, *y*−1/2, −*z*+1; (vi) −*x*+1, −*y*+1, −*z*+1; (vii) −*x*+1, −*y*+1, −*z*; (viii) −*x*, −*y*+1, −*z*+1; (ix) −*x*, *y*−1/2, −*z*; (x) −*x*, *y*+1/2, −*z*; (xi) *x*+1, −*y*+1/2, *z*; (xii) *x*−1, *y*, *z*.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N6*A*—H6*A*···O9*A*^{iv}	0.88 (3)	2.05 (3)	2.9207 (19)	172 (2)
N6*A*—H6*B*···O9*B*^{vi}	0.83 (3)	2.26 (3)	3.074 (2)	164 (2)
N7*A*—H7*A*···O9*B*^{ii}	0.87 (3)	1.93 (3)	2.8033 (18)	177 (2)
N7*A*—H7*A*···O9*B*^{vi}	0.87 (3)	1.93 (3)	2.8033 (18)	177 (2)
N6*B*—H6*C*···N5*A*^{vii}	0.88 (2)	2.31 (2)	3.189 (2)	175 (2)
N6*B*—H6*D*···O9*A*^{iii}	0.85 (3)	2.31 (3)	2.8121 (19)	118 (2)
N6*B*—H6*D*···N2*A*^{iii}	0.85 (3)	2.20 (3)	3.0387 (19)	166 (3)
N7*B*—H7*B*···O1*A*^{vii}	0.91 (3)	2.24 (3)	3.0354 (17)	145 (2)
N7*B*—H7*B*···N5*A*^{vii}	0.91 (3)	2.32 (3)	3.2302 (19)	179 (2)
C8*A*—H8*A*···O1*B*^{viii}	0.95	2.32	3.266 (2)	175
C8*B*—H8*B*···N5*B*^{xi}	0.95	2.55	3.489 (2)	170

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