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Crystal structure and Hirshfeld surface analysis of 2,5-diimino-8a-methyl-4,9-bis(4-methylphenyl)-7-oxo-6-phenyl-decahydro-2*H*-3,8-methanopyrano-[3,2-*c*]pyridine-3,4a-dicarbonitrile *N*,*N*-dimethylformamide monosolvate

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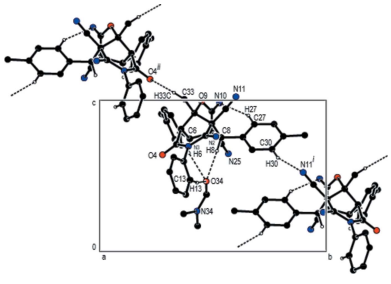
In the title compound, $C_{32}H_{29}N_5O_2\cdot C_3H_7NO$, the bicyclo[3.3.1]nonane ring system adopts a half-chair/twist-boat conformation, with the phenyl rings in equatorial orientations with respect to the piperidine ring. The two oxane rings of the 2-oxabicyclo[2.2.2]octane ring system exhibit a distorted boat conformation. Intermolecular C—H···O and C—H···N hydrogen bonds connect the molecules in the crystal, generating layers extending parallel to (100). These layers are connected by C—H···π interactions. A Hirshfeld surface analysis was performed to quantify the contributions of the different intermolecular interactions, indicating that the most important contributions to the crystal packing are from H···H (52.5%), N···H/H···N (19.2%), C···H/H···C (18.8%) and O···H/H···O (8.3%) interactions.

1. Chemical context

Different C—C, C—N, and C—O bond-formation methods play important roles in various organic synthesis directions (Aliyeva *et al.*, 2011; Zubkov *et al.*, 2018; Viswanathan *et al.*, 2019; Mamedov *et al.*, 2022). Heterocyclic systems, especially those comprising the pyrano[3,2-*c*]pyridine scaffold, are present in many natural or synthetic products with a wide spectrum of biological properties, such as antitumor, antitubercular, cholinesterase inhibitor and anti-diabetic activities (Mamedov *et al.*, 2019; Kumari *et al.*, 2018). One of the most effective synthetic approaches to these polyfunctional heterocyclic systems is a Michael addition of active methylene compounds at the ylidene malononitrile functionality (Girgis *et al.*, 2015). In a recent study (Mamedov *et al.*, 2019), we found



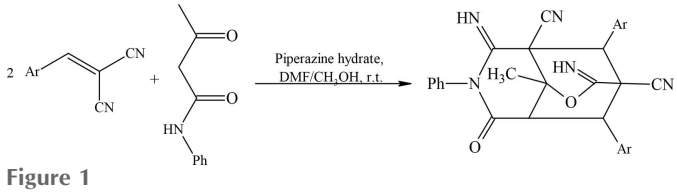


Figure 1
Chemical scheme for the one-pot synthesis of tricyclic pyrano[3,2-*c*]-pyridine derivatives.

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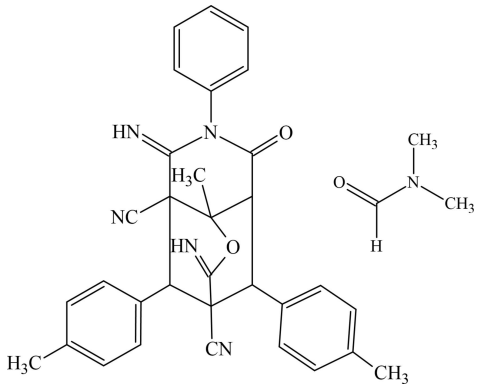
that the reaction of two moles of arylidene malononitriles with acetoacetanilide in the presence of piperazine hydrate leads to the formation of novel tricyclic pyrano[3,2-*c*]pyridine derivatives at room temperature (Fig. 1).

In this context and with respect to our on-going structural studies (Naghiyev *et al.*, 2020, 2021, 2022; Khalilov *et al.*, 2022), we report here the crystal structure and Hirshfeld surface analysis of 2,5-diimino-8a-methyl-4,9-bis(4-methylphenyl)-7-oxo-6-phenyl-decahydro-2*H*-3,8-methanopyrano[3,2-*c*]pyridine-3,4a-dicarbonitrile *N*,*N*-dimethylformamide monosolvate, $C_{32}H_{29}N_5O_2\cdot C_3H_7NO$.



2. Structural commentary

The molecular structure of the title compound is displayed in Fig. 2. The molecular conformation is stabilized by an intramolecular C—H···N hydrogen bond (Table 1) and consolidated by intermolecular C—H···O interactions involving the *N*,*N*-dimethylformamide solvent molecule (Fig. 2). As shown in Fig. 3, the bicyclo[3.3.1]nonane ring system (C2/N3/C4–C8/C1/C9) adopts a half-chair/twist-boat conformation; the puckering parameters (Cremer & Pople, 1975) are Q_T = 0.529 (2) Å, θ = 53.0 (2)°, φ = 160.1 (3)° for the (N3/C2/C1/C9/C5/C4) ring, and Q_T = 0.889 (2) Å, θ = 89.21 (13)°, φ = 289.11 (14)° for the (C1/C8/C7/C6/C5/C9) ring. The phenyl rings (C12–C17, C18–C23 and C26–C31) are in equatorial orientations with respect to the piperidine ring (C1/C2/N3/C4/C5/C9). The two oxane rings (O9/C9/C1/C8/C7/C10 and O9/C9/C5/C6/C7/C10) of the 2-oxabicyclo[2.2.2]octane ring system (C10/O9/C9/C1/C8/C7/C6/C5) exhibit a distorted boat conformation with puckering parameters Q_T = 0.799 (2) Å, θ = 91.88 (14)°, φ = 247.89 (15)° for the O9/C9/C1/C8C7/C10 ring, and Q_T = 0.826 (2) Å, θ = 96.04 (14)°, φ = 50.59 (15)° for the O9/C9/C5/C6/C7/C10 ring.

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

*Cg*7 is the centroid of the C26–C31 benzene ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H6···O34	1.00	2.44	3.297 (3)	143
C8—H8···O34	1.00	2.34	3.241 (3)	149
C13—H13···O34	0.95	2.47	3.373 (3)	159
C27—H27···N10	0.95	2.56	3.432 (3)	152
C30—H30···N11^{i}	0.95	2.61	3.515 (3)	160
C33—H33*C*···O4^{ii}	0.98	2.48	3.447 (3)	170
C24—H24*C*···*Cg*7^{iii}	0.98	2.84	3.715 (2)	148

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

3. Supramolecular features and Hirshfeld surface analysis

In the crystal, intermolecular C—H···O and C—H···N hydrogen bonds (Table 1) link individual molecules, forming layers parallel to (100) (Fig. 4). These layers are connected by C—H···π interactions (Fig. 5). Interestingly, the imine C=N—H groups are not involved in hydrogen-bonding interactions.

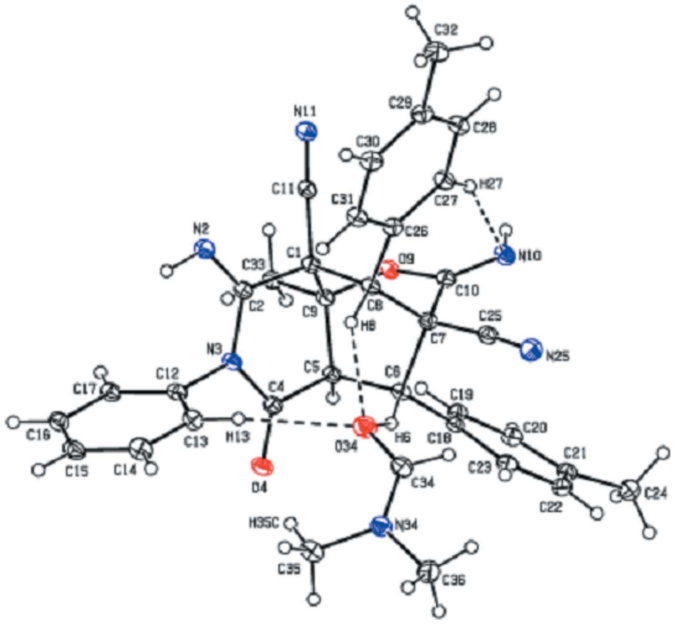


Figure 2
The molecular entities of the title compound, showing the atom labelling and displacement ellipsoids drawn at the 30% probability level. C—H···O and C—H···N hydrogen bonds are indicated by dashed lines.

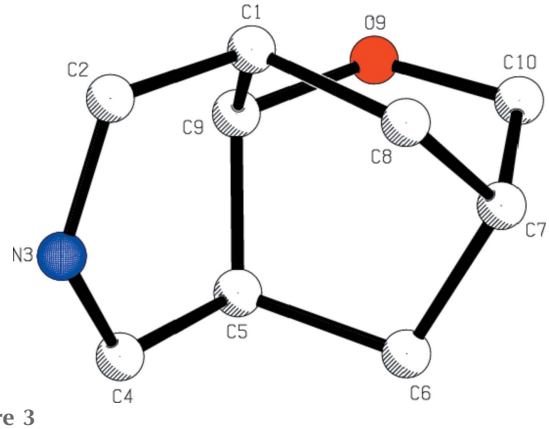


Figure 3
View of the octahydro-2*H*-3,8-methanopyrano[3,2-*c*]pyridine ring sytem of the title compound.

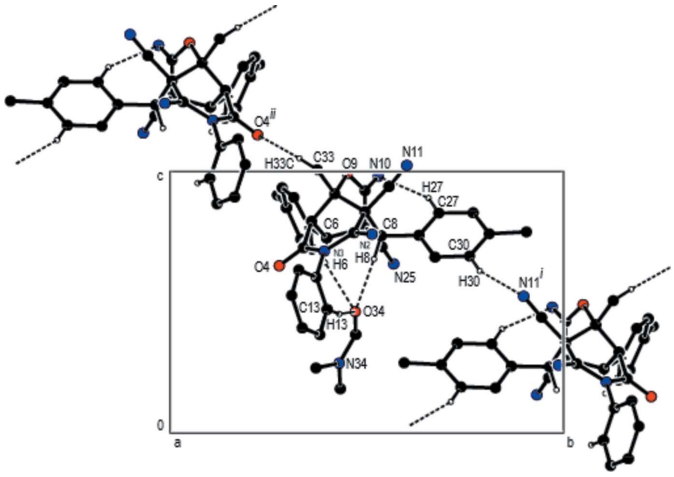


Figure 4
A partial view of the crystal packing along the *a* axis of the title compound with C—H···O and C—H···N hydrogen bonds indicated (dashed lines). [Symmetry codes: (i) $x, -y+\frac{1}{2}, z-\frac{3}{2}$; (ii) $x, -y-\frac{1}{2}, z-\frac{1}{2}$].

A Hirshfeld surface analysis was performed to quantify the intermolecular interactions; the accompanying two-dimensional fingerprint plots were obtained using *CrystalExplorer17* (Turner *et al.*, 2017). The Hirshfeld surface mapped over d_{norm} using a standard surface resolution with a fixed colour scale of −0.1713 (red) to 1.4361 (blue) a.u. is shown in Fig. 6. The shorter and longer contacts are indicated as red and blue spots, respectively, on the Hirshfeld surfaces, and contacts with distances approximately equal to the sum of the van der Waals

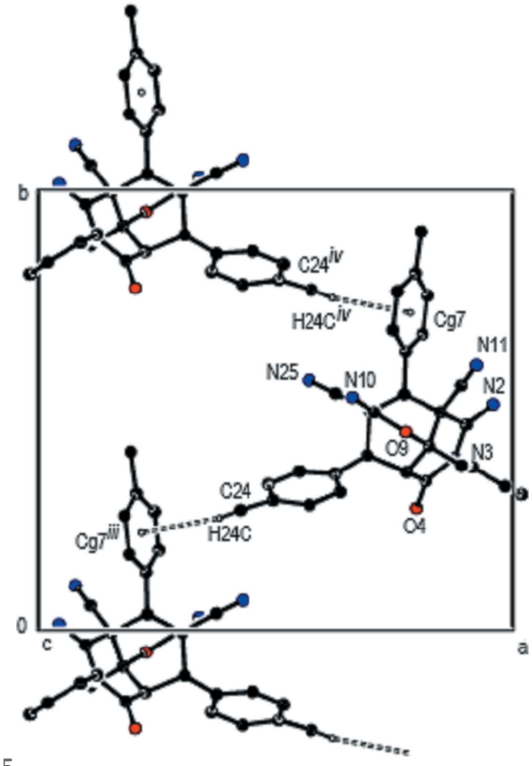


Figure 5
A general view of the packing in the unit cell of the title compound with C—H···π interactions indicated (dashed lines). [Symmetry codes: (iii) $-x+1, y-\frac{1}{2}, -z+\frac{3}{2}$; (iv) $-x+1, y+\frac{1}{2}, -z+\frac{3}{2}$].

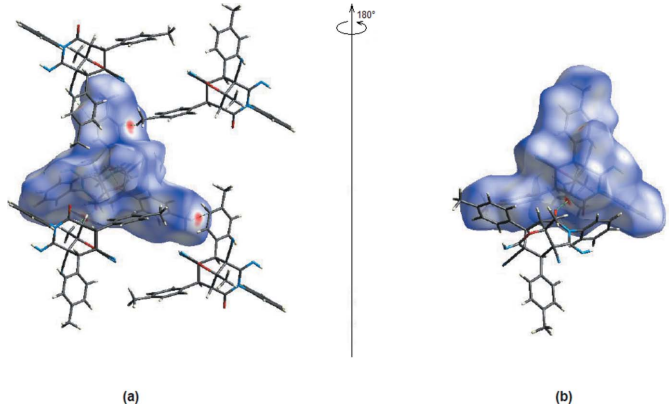


Figure 6
(*a*) Front and (*b*) back sides of the three-dimensional Hirshfeld surface of the title compound mapped over d_{norm}, with a fixed colour scale of −0.1713 to 1.4361 a.u..

radii are represented as white spots. The most important red spots on the d_{norm} surface represent the aforementioned C—H···O and C—H···N interactions (Tables 1, 2).

Fig. 7 depicts the two-dimensional fingerprint plots of (d_i, d_e) points from all the contacts contributing to the Hirshfeld surface analysis in normal mode for all atoms. The most

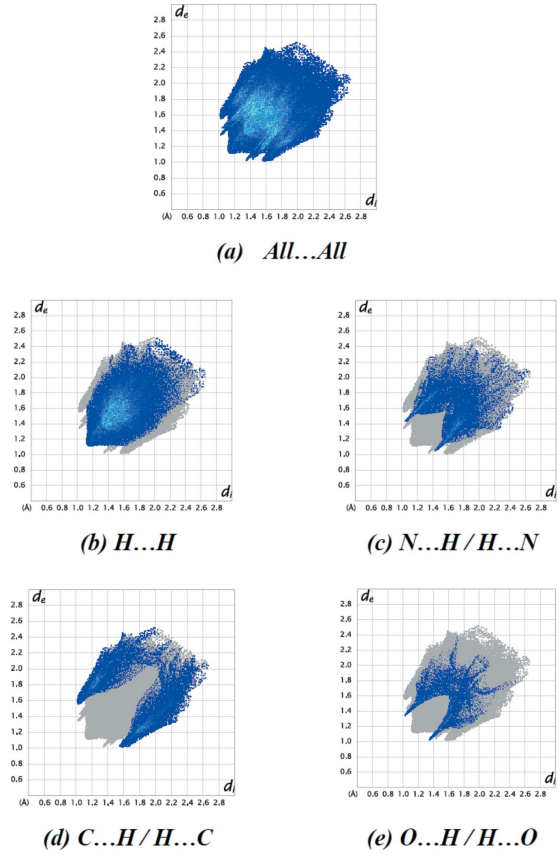


Figure 7
The two-dimensional fingerprint plots of the title compound, showing (*a*) all interactions, and delineated into (*b*) H···H, (*c*) N···H/H···N, (*d*) C···H/H···C and (*e*) O···H/H···O interactions. [d_e and d_i represent the distances from a point on the Hirshfeld surface to the nearest atoms outside (external) and inside (internal) the surface, respectively].

Table 2
Summary of short interatomic contacts (Å) in the title compound.

Atoms	Distance	Symmetry code
O4···H33*C*	2.48	$x, \frac{1}{2}-y, -\frac{1}{2}+z$
H10*N*···H35*A*	2.35	$x, y, 1+z$
H10*N*···H32*B*	2.52	$x, \frac{3}{2}-y, \frac{1}{2}+z$
H33*A*···N2	2.70	$2-x, 1-y, 2-z$
H15···N2	2.92	$2-x, 1-y, 1-z$
H24*A*···N10	2.82	$1-x, 1-y, 2-z$
C29···H16	2.85	$2-x, \frac{1}{2}+y, \frac{3}{2}-z$
C28···H24*C*	2.68	$1-x, \frac{1}{2}+y, \frac{3}{2}-z$
N25···H36*C*	2.77	$1-x, 1-y, 1-z$
H13···H35*C*	2.29	x, y, z
C18···H35*B*	2.91	$x, \frac{1}{2}-y, \frac{1}{2}+z$
H32*B*···C34	3.04	$x, \frac{3}{2}-y, \frac{1}{2}+z$

important intermolecular interactions are H···H contacts, contributing 52.5% to the overall crystal packing. Other interactions and their respective contributions are N···H/H···N (19.2%), C···H/H···C (18.8%), O···H/H···O (8.3%), N···N (0.6%), C···N/N···C (0.3%), C···C (0.2%) and C···O/O···C (0.1%), respectively.

The Hirshfeld surface study verifies the significance of H-atom interactions in the packing formation. The contributions of H···H and N···H/H···N interactions imply that van der Waals interactions are important in the crystal packing (Hathwar *et al.*, 2015).

4. Database survey

The five most similar compounds found in a search of the Cambridge Structural Database (CSD, Version 5.42, update of September 2021; Groom *et al.*, 2016) for the bicyclo [3.3.1]nonane ring system are: 7-*tert*-butyl-*N*-methyl-2,4-diphenyl-3-azabicyclo[3.3.1]nonane (**I**) (Kumaran *et al.*, 1999), *N*-acetyl-2,4-diphenyl-3-azabicyclo[3.3.1]nonane (**II**) (Kumaran *et al.*, 1999), *N*-methyl-2,4-bis(2- methylphenyl)-3-azabicyclo[3.3.1]nonan-9-ol (**III**) (Kumaran *et al.*, 1999), 3-azabicyclo[3.3.1]nonane- 2,4-dione (form 2) (**IV**) (Hulme *et al.*, 2006) and 2,4-bis(furan-2-yl)-1,5-dimethyl-3-azabicyclo [3.3.1]nonan-9-one (**V**) (Venkateswaramoorthi *et al.*, 2013).

Compounds (**I**) and (**III**) crystallize in monoclinic space groups ($P2_1/c$, $Z = 4$, and $P2_1/n$, $Z = 4$, respectively), whereas (**II**) is orthorhombic (*Pbca*, $Z = 8$). In each of the three structures, the bicyclic ring system adopts a chair/chair conformation and the phenyl rings are in equatorial orientations with respect to the piperidine ring. In (**II**), apart from van der Waals forces, only weak intermolecular C—H···O-type interactions are involved in the packing.

The structure of (**IV**) has monoclinic symmetry ($P2_1/c$, $Z = 8$) and has two molecules in the asymmetric unit. A $C_2^2(8)$ chain motif (Bernstein *et al.*, 1995) is formed *via* N—H···O hydrogen bonds.

In (**V**), which likewise is monoclinic ($C2/c$, $Z = 8$), the bicyclic ring system adopts a twin-chair conformation. The two methyl groups attached to the bicycle are in an equatorial orientation for both rings. In the crystal, very long N—H···O hydrogen bonds connect the molecules into a chain perpendicular to [010].

Table 3
Experimental details.

Crystal data	
Chemical formula	$C_{32}H_{27}N_5O_2\cdot C_3H_7NO$
M_r	586.68
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	100
a, b, c (Å)	17.6747 (3), 15.7656 (2), 10.9086 (2)
β (°)	105.666 (2)
V (Å^3)	2926.79 (9)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	0.70
Crystal size (mm)	0.14 × 0.11 × 0.08
Data collection	
Diffractometer	XtaLAB Synergy, Dualflex, HyPix
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2021)
T_{min}, T_{max}	0.900, 0.936
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	31226, 6140, 5275
R_{int}	0.051
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.638
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.059, 0.166, 1.08
No. of reflections	6140
No. of parameters	408
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.34, −0.36

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

5. Synthesis and crystallization

The title compound was synthesized using a previously reported procedure (Mamedov *et al.*, 2019). Colourless crystals were obtained upon recrystallization from an ethanol/water (3:1 *v*/*v*) solution.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. All C-bound H atoms were placed at calculated positions and refined using a riding model, with C—H = 0.95–1.00 Å, and with U_{iso}(H) = 1.2 or 1.5U_{eq}(C). The N-bound H atoms were located from difference-Fourier maps and refined with free atomic coordinates and $U_{iso} = 1.2U_{eq}$(N).

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Author contributions are as follows. Conceptualization, ANK and IGM; methodology, ANK, FNN and IGM; investigation, ANK, MA and APN; writing (original draft), MA and ANK; writing (review and editing of the manuscript), MA and ANK; visualization, MA, ANK and IGM; funding acquisition, VNK, AB and ANK; resources, AB, VNK and APN; supervision, ANK and MA.

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supporting information

Acta Cryst. (2023). E**79**, 254-258 [https://doi.org/10.1107/S2056989023001718]

Crystal structure and Hirshfeld surface analysis of 2,5-diimino-8a-methyl-4,9-bis(4-methylphenyl)-7-oxo-6-phenyl-decahydro-2*H*-3,8-methanopyrano[3,2-*c*]pyridine-3,4a-dicarbonitrile *N*,*N*-dimethylformamide monosolvate

Farid N. Naghiyev, Victor N. Khrustalev, Anton P. Novikov, Mehmet Akkurt, Ali N. Khalilov, Ajaya Bhattarai and İbrahim G. Mamedov

Computing details

Data collection: *CrysAlis PRO* (Rigaku OD, 2021); cell refinement: *CrysAlis PRO* (Rigaku OD, 2021); data reduction: *CrysAlis PRO* (Rigaku OD, 2021); 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).

4,10-Diimino-8-methyl-2,11-bis(4-methylphenyl)-6-oxo-5-phenyl-9-oxa-5-azatricyclo[5.3.1.0^{3,8}]undecane-1,3-dicarbonitrile *N*,*N*-dimethylformamide monosolvate

Crystal data

$C_{32}H_{27}N_5O_2\cdot C_3H_7NO$
M_r = 586.68
Monoclinic, $P2_1/c$
a = 17.6747 (3) Å
b = 15.7656 (2) Å
c = 10.9086 (2) Å
β = 105.666 (2)°
V = 2926.79 (9) Å^3
Z = 4
$F(000)$ = 1240
D_x = 1.331 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54184 Å
Cell parameters from 19771 reflections
θ = 3.8–79.0°
μ = 0.70 mm^{-1}
T = 100 K
Prism, colourless
0.14 × 0.11 × 0.08 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} = 0.900, T_{max} = 0.936
31226 measured reflections
6140 independent reflections
5275 reflections with $I > 2\sigma(I)$
R_{int} = 0.051
θ_{max} = 79.5°, θ_{min} = 3.8°
h = −22→21
k = −20→19
l = −12→13

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.166
S = 1.08
6140 reflections
408 parameters
0 restraints
Hydrogen site location: mixed

H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0745P)^2 + 3.3477P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.34$ e Å^{-3}
$\Delta\rho_{min} = -0.36$ 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.

Refinement. Owing to poor agreement between observed and calculated intensities, twenty-three outliers ($\bar{2}$ 5 1, $\bar{3}$ 8 1, $\bar{1}$ 8 9, $\bar{12}$ 2 8, $\bar{1}$ 8 1, 4 0 8, $\bar{2}$ 1 1, $\bar{4}$ 12 10, 4 2 7, $\bar{5}$ 12 8, 1 1 7, $\bar{3}$ 6 8, $\bar{6}$ 3 9, $\bar{1}$ 9 9, 12 11 1, $\bar{2}$ 9 9, $\bar{1}$ 9 7, $\bar{5}$ 3 9, $\bar{5}$ 14 7, 3 6 1, 0 1 7, $\bar{12}$ 2 7, and 1 11 8) were omitted in the final cycles of refinement.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.84688 (12)	0.49523 (12)	0.84606 (19)	0.0192 (4)
C2	0.90039 (12)	0.46714 (13)	0.76567 (19)	0.0198 (4)
C4	0.81629 (12)	0.33885 (13)	0.70834 (19)	0.0206 (4)
C5	0.77485 (12)	0.35958 (13)	0.81000 (19)	0.0194 (4)
H5	0.766607	0.305061	0.851447	0.023*
C6	0.69240 (12)	0.39782 (13)	0.74590 (19)	0.0203 (4)
H6	0.682604	0.393814	0.651413	0.024*
C7	0.69769 (12)	0.49505 (13)	0.78496 (19)	0.0200 (4)
C8	0.77028 (12)	0.53623 (13)	0.75358 (19)	0.0195 (4)
H8	0.769058	0.518255	0.665155	0.023*
C9	0.82223 (12)	0.41853 (13)	0.91434 (19)	0.0198 (4)
C10	0.70680 (12)	0.49526 (13)	0.9264 (2)	0.0207 (4)
C11	0.88965 (12)	0.55627 (13)	0.94255 (19)	0.0201 (4)
C12	0.91367 (12)	0.37153 (13)	0.5957 (2)	0.0214 (4)
C13	0.87775 (13)	0.39897 (14)	0.4729 (2)	0.0261 (5)
H13	0.829930	0.429983	0.455287	0.031*
C14	0.91246 (15)	0.38060 (16)	0.3761 (2)	0.0305 (5)
H14	0.888170	0.398723	0.291590	0.037*
C15	0.98255 (14)	0.33583 (15)	0.4026 (2)	0.0283 (5)
H15	1.006297	0.323451	0.336214	0.034*
C16	1.01812 (13)	0.30904 (14)	0.5263 (2)	0.0271 (5)
H16	1.066067	0.278253	0.544171	0.033*
C17	0.98380 (13)	0.32713 (13)	0.6236 (2)	0.0241 (4)
H17	1.008099	0.309285	0.708266	0.029*
C18	0.62485 (12)	0.35539 (13)	0.7832 (2)	0.0208 (4)
C19	0.63465 (13)	0.31443 (13)	0.9005 (2)	0.0225 (4)
H19	0.685990	0.306811	0.955333	0.027*
C20	0.57009 (13)	0.28484 (14)	0.9374 (2)	0.0241 (4)
H20	0.578280	0.256282	1.016577	0.029*
C21	0.49370 (13)	0.29599 (14)	0.8612 (2)	0.0248 (5)
C22	0.48456 (13)	0.33204 (14)	0.7412 (2)	0.0249 (5)
H22	0.433380	0.336973	0.684802	0.030*

C23	0.54892 (13)	0.36093 (13)	0.7026 (2)	0.0231 (4)
H23	0.541005	0.384761	0.620081	0.028*
C24	0.42432 (13)	0.27319 (15)	0.9096 (2)	0.0288 (5)
H24A	0.408264	0.322797	0.950610	0.043*
H24B	0.438846	0.226951	0.971608	0.043*
H24C	0.380636	0.254957	0.838265	0.043*
C25	0.62564 (13)	0.53826 (13)	0.7117 (2)	0.0231 (4)
C26	0.77331 (12)	0.63271 (13)	0.75573 (19)	0.0213 (4)
C27	0.74616 (13)	0.68268 (13)	0.8408 (2)	0.0229 (4)
H27	0.721083	0.656657	0.897947	0.028*
C28	0.75561 (13)	0.77005 (14)	0.8423 (2)	0.0244 (4)
H28	0.736015	0.802987	0.899962	0.029*
C29	0.79307 (13)	0.81081 (14)	0.7616 (2)	0.0242 (4)
C30	0.81945 (13)	0.76077 (14)	0.6766 (2)	0.0251 (5)
H30	0.844772	0.786878	0.619812	0.030*
C31	0.80946 (13)	0.67318 (14)	0.6730 (2)	0.0238 (4)
H31	0.827533	0.640525	0.613376	0.029*
C32	0.80575 (15)	0.90535 (14)	0.7689 (2)	0.0301 (5)
H32A	0.852432	0.918575	0.838280	0.045*
H32B	0.759739	0.933163	0.784828	0.045*
H32C	0.813314	0.925827	0.688169	0.045*
C33	0.89004 (12)	0.37404 (13)	1.0063 (2)	0.0218 (4)
H33A	0.919202	0.414849	1.069304	0.033*
H33B	0.925089	0.349923	0.959485	0.033*
H33C	0.869776	0.328506	1.049816	0.033*
C34	0.63579 (14)	0.47173 (15)	0.3770 (2)	0.0275 (5)
H34	0.593630	0.505419	0.388302	0.033*
C35	0.68357 (15)	0.37063 (15)	0.2489 (2)	0.0300 (5)
H35A	0.709455	0.394672	0.187861	0.045*
H35B	0.658547	0.316752	0.215915	0.045*
H35C	0.722664	0.360780	0.330382	0.045*
C36	0.54932 (14)	0.43254 (18)	0.1702 (2)	0.0338 (5)
H36A	0.521478	0.378714	0.169526	0.051*
H36B	0.558662	0.441861	0.086657	0.051*
H36C	0.517414	0.479056	0.188991	0.051*
N2	0.95780 (11)	0.51308 (12)	0.75995 (18)	0.0242 (4)
H2N	0.9840 (16)	0.4923 (18)	0.702 (3)	0.029*
N3	0.87658 (10)	0.39156 (11)	0.69547 (16)	0.0205 (4)
N10	0.66000 (11)	0.52902 (12)	0.98087 (19)	0.0252 (4)
H10N	0.6751 (16)	0.5206 (18)	1.071 (3)	0.030*
N11	0.92084 (11)	0.60155 (12)	1.02287 (17)	0.0250 (4)
N25	0.57038 (11)	0.56806 (13)	0.64654 (19)	0.0298 (4)
N34	0.62423 (11)	0.42955 (12)	0.26736 (18)	0.0265 (4)
O4	0.79621 (9)	0.27759 (10)	0.63952 (15)	0.0270 (4)
O9	0.77226 (8)	0.45054 (9)	0.99082 (13)	0.0202 (3)
O34	0.69653 (10)	0.47051 (11)	0.46440 (15)	0.0332 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0237 (10)	0.0151 (9)	0.0192 (9)	−0.0017 (7)	0.0064 (8)	−0.0003 (7)
C2	0.0234 (10)	0.0172 (9)	0.0190 (9)	0.0005 (8)	0.0063 (8)	0.0001 (8)
C4	0.0235 (10)	0.0171 (9)	0.0218 (10)	0.0008 (8)	0.0069 (8)	0.0007 (8)
C5	0.0240 (10)	0.0146 (9)	0.0209 (10)	−0.0016 (7)	0.0080 (8)	−0.0012 (7)
C6	0.0245 (10)	0.0162 (9)	0.0198 (10)	0.0002 (8)	0.0052 (8)	−0.0017 (7)
C7	0.0219 (10)	0.0168 (9)	0.0210 (10)	0.0003 (8)	0.0052 (8)	0.0000 (8)
C8	0.0248 (10)	0.0178 (9)	0.0166 (9)	−0.0004 (8)	0.0064 (8)	−0.0003 (7)
C9	0.0231 (10)	0.0172 (9)	0.0207 (10)	0.0000 (8)	0.0086 (8)	−0.0010 (8)
C10	0.0239 (10)	0.0148 (9)	0.0235 (10)	−0.0018 (7)	0.0066 (8)	−0.0002 (8)
C11	0.0242 (10)	0.0164 (9)	0.0209 (10)	0.0007 (8)	0.0080 (8)	0.0000 (8)
C12	0.0273 (10)	0.0176 (9)	0.0210 (10)	−0.0034 (8)	0.0092 (8)	−0.0031 (8)
C13	0.0284 (11)	0.0244 (11)	0.0260 (11)	0.0021 (9)	0.0081 (9)	0.0000 (9)
C14	0.0384 (13)	0.0314 (12)	0.0233 (11)	−0.0003 (10)	0.0110 (9)	0.0015 (9)
C15	0.0363 (12)	0.0256 (11)	0.0282 (11)	−0.0051 (9)	0.0179 (9)	−0.0069 (9)
C16	0.0278 (11)	0.0213 (10)	0.0346 (12)	−0.0010 (9)	0.0126 (9)	−0.0039 (9)
C17	0.0282 (11)	0.0184 (10)	0.0262 (11)	−0.0007 (8)	0.0082 (8)	−0.0009 (8)
C18	0.0242 (10)	0.0151 (9)	0.0237 (10)	−0.0001 (8)	0.0078 (8)	−0.0037 (8)
C19	0.0243 (10)	0.0196 (10)	0.0224 (10)	−0.0005 (8)	0.0046 (8)	−0.0012 (8)
C20	0.0303 (11)	0.0212 (10)	0.0216 (10)	−0.0029 (8)	0.0083 (9)	−0.0013 (8)
C21	0.0282 (11)	0.0191 (10)	0.0285 (11)	−0.0030 (8)	0.0100 (9)	−0.0049 (8)
C22	0.0238 (10)	0.0216 (10)	0.0274 (11)	−0.0006 (8)	0.0035 (8)	−0.0026 (8)
C23	0.0298 (11)	0.0178 (10)	0.0213 (10)	−0.0009 (8)	0.0062 (8)	−0.0003 (8)
C24	0.0274 (11)	0.0276 (12)	0.0328 (12)	−0.0032 (9)	0.0103 (9)	−0.0026 (9)
C25	0.0265 (11)	0.0188 (10)	0.0254 (11)	−0.0018 (8)	0.0093 (9)	−0.0021 (8)
C26	0.0241 (10)	0.0181 (10)	0.0203 (10)	0.0002 (8)	0.0037 (8)	0.0018 (8)
C27	0.0287 (11)	0.0184 (10)	0.0228 (10)	0.0001 (8)	0.0088 (8)	0.0012 (8)
C28	0.0307 (11)	0.0194 (10)	0.0223 (10)	0.0020 (8)	0.0059 (9)	−0.0016 (8)
C29	0.0282 (11)	0.0189 (10)	0.0224 (10)	−0.0004 (8)	0.0018 (8)	0.0019 (8)
C30	0.0324 (11)	0.0199 (10)	0.0230 (10)	−0.0028 (9)	0.0073 (9)	0.0034 (8)
C31	0.0300 (11)	0.0210 (10)	0.0213 (10)	0.0004 (8)	0.0084 (8)	0.0003 (8)
C32	0.0392 (13)	0.0185 (10)	0.0317 (12)	−0.0009 (9)	0.0076 (10)	0.0021 (9)
C33	0.0259 (10)	0.0173 (9)	0.0220 (10)	−0.0006 (8)	0.0060 (8)	0.0014 (8)
C34	0.0314 (11)	0.0279 (11)	0.0243 (11)	0.0010 (9)	0.0094 (9)	−0.0010 (9)
C35	0.0376 (13)	0.0254 (11)	0.0277 (11)	0.0027 (9)	0.0100 (10)	−0.0009 (9)
C36	0.0295 (12)	0.0434 (14)	0.0277 (12)	0.0001 (10)	0.0063 (9)	−0.0046 (10)
N2	0.0280 (9)	0.0221 (9)	0.0245 (9)	−0.0027 (7)	0.0105 (8)	−0.0021 (7)
N3	0.0255 (9)	0.0163 (8)	0.0217 (8)	−0.0020 (7)	0.0098 (7)	−0.0027 (7)
N10	0.0311 (10)	0.0216 (9)	0.0260 (10)	−0.0001 (7)	0.0131 (8)	0.0001 (7)
N11	0.0283 (9)	0.0212 (9)	0.0255 (9)	−0.0004 (7)	0.0073 (7)	−0.0010 (7)
N25	0.0291 (10)	0.0244 (10)	0.0346 (11)	0.0011 (8)	0.0061 (8)	0.0030 (8)
N34	0.0288 (10)	0.0263 (10)	0.0241 (9)	0.0010 (8)	0.0064 (8)	−0.0018 (7)
O4	0.0322 (8)	0.0205 (7)	0.0307 (8)	−0.0034 (6)	0.0126 (7)	−0.0073 (6)
O9	0.0241 (7)	0.0187 (7)	0.0191 (7)	0.0014 (5)	0.0081 (6)	0.0003 (5)
O34	0.0358 (9)	0.0365 (9)	0.0253 (8)	0.0032 (7)	0.0049 (7)	−0.0042 (7)

Geometric parameters (Å, º)

C1—C11	1.475 (3)	C20—C21	1.392 (3)
C1—C2	1.519 (3)	C20—H20	0.9500
C1—C9	1.543 (3)	C21—C22	1.396 (3)
C1—C8	1.591 (3)	C21—C24	1.504 (3)
C2—N2	1.262 (3)	C22—C23	1.392 (3)
C2—N3	1.418 (3)	C22—H22	0.9500
C4—O4	1.216 (3)	C23—H23	0.9500
C4—N3	1.388 (3)	C24—H24A	0.9800
C4—C5	1.520 (3)	C24—H24B	0.9800
C5—C9	1.532 (3)	C24—H24C	0.9800
C5—C6	1.557 (3)	C25—N25	1.143 (3)
C5—H5	1.0000	C26—C31	1.393 (3)
C6—C18	1.517 (3)	C26—C27	1.397 (3)
C6—C7	1.587 (3)	C27—C28	1.387 (3)
C6—H6	1.0000	C27—H27	0.9500
C7—C25	1.475 (3)	C28—C29	1.393 (3)
C7—C10	1.507 (3)	C28—H28	0.9500
C7—C8	1.556 (3)	C29—C30	1.391 (3)
C8—C26	1.522 (3)	C29—C32	1.506 (3)
C8—H8	1.0000	C30—C31	1.391 (3)
C9—O9	1.459 (2)	C30—H30	0.9500
C9—C33	1.512 (3)	C31—H31	0.9500
C10—N10	1.259 (3)	C32—H32A	0.9800
C10—O9	1.375 (2)	C32—H32B	0.9800
C11—N11	1.149 (3)	C32—H32C	0.9800
C12—C17	1.384 (3)	C33—H33A	0.9800
C12—C13	1.388 (3)	C33—H33B	0.9800
C12—N3	1.449 (3)	C33—H33C	0.9800
C13—C14	1.387 (3)	C34—O34	1.229 (3)
C13—H13	0.9500	C34—N34	1.335 (3)
C14—C15	1.387 (3)	C34—H34	0.9500
C14—H14	0.9500	C35—N34	1.455 (3)
C15—C16	1.392 (3)	C35—H35A	0.9800
C15—H15	0.9500	C35—H35B	0.9800
C16—C17	1.387 (3)	C35—H35C	0.9800
C16—H16	0.9500	C36—N34	1.456 (3)
C17—H17	0.9500	C36—H36A	0.9800
C18—C23	1.395 (3)	C36—H36B	0.9800
C18—C19	1.401 (3)	C36—H36C	0.9800
C19—C20	1.389 (3)	N2—H2N	0.94 (3)
C19—H19	0.9500	N10—H10N	0.95 (3)
C11—C1—C2	108.85 (17)	C21—C20—H20	119.2
C11—C1—C9	108.90 (17)	C20—C21—C22	117.3 (2)
C2—C1—C9	110.55 (16)	C20—C21—C24	120.8 (2)
C11—C1—C8	111.83 (16)	C22—C21—C24	121.8 (2)

C2—C1—C8	107.95 (16)	C23—C22—C21	121.3 (2)
C9—C1—C8	108.76 (16)	C23—C22—H22	119.3
N2—C2—N3	125.53 (19)	C21—C22—H22	119.3
N2—C2—C1	119.71 (19)	C22—C23—C18	120.9 (2)
N3—C2—C1	114.63 (17)	C22—C23—H23	119.5
O4—C4—N3	121.14 (19)	C18—C23—H23	119.5
O4—C4—C5	120.22 (18)	C21—C24—H24A	109.5
N3—C4—C5	118.64 (17)	C21—C24—H24B	109.5
C4—C5—C9	113.46 (17)	H24A—C24—H24B	109.5
C4—C5—C6	109.41 (16)	C21—C24—H24C	109.5
C9—C5—C6	110.87 (16)	H24A—C24—H24C	109.5
C4—C5—H5	107.6	H24B—C24—H24C	109.5
C9—C5—H5	107.6	N25—C25—C7	174.4 (2)
C6—C5—H5	107.6	C31—C26—C27	118.15 (19)
C18—C6—C5	114.69 (17)	C31—C26—C8	117.91 (19)
C18—C6—C7	110.33 (16)	C27—C26—C8	123.83 (19)
C5—C6—C7	105.86 (16)	C28—C27—C26	120.4 (2)
C18—C6—H6	108.6	C28—C27—H27	119.8
C5—C6—H6	108.6	C26—C27—H27	119.8
C7—C6—H6	108.6	C27—C28—C29	121.8 (2)
C25—C7—C10	113.04 (18)	C27—C28—H28	119.1
C25—C7—C8	109.31 (17)	C29—C28—H28	119.1
C10—C7—C8	110.95 (17)	C30—C29—C28	117.5 (2)
C25—C7—C6	108.74 (16)	C30—C29—C32	121.6 (2)
C10—C7—C6	105.03 (16)	C28—C29—C32	120.8 (2)
C8—C7—C6	109.64 (16)	C29—C30—C31	121.2 (2)
C26—C8—C7	116.18 (17)	C29—C30—H30	119.4
C26—C8—C1	112.08 (16)	C31—C30—H30	119.4
C7—C8—C1	107.58 (16)	C30—C31—C26	120.9 (2)
C26—C8—H8	106.8	C30—C31—H31	119.6
C7—C8—H8	106.8	C26—C31—H31	119.6
C1—C8—H8	106.8	C29—C32—H32A	109.5
O9—C9—C33	105.95 (16)	C29—C32—H32B	109.5
O9—C9—C5	109.93 (16)	H32A—C32—H32B	109.5
C33—C9—C5	112.84 (17)	C29—C32—H32C	109.5
O9—C9—C1	107.35 (16)	H32A—C32—H32C	109.5
C33—C9—C1	114.04 (17)	H32B—C32—H32C	109.5
C5—C9—C1	106.61 (16)	C9—C33—H33A	109.5
N10—C10—O9	123.02 (19)	C9—C33—H33B	109.5
N10—C10—C7	125.6 (2)	H33A—C33—H33B	109.5
O9—C10—C7	111.38 (17)	C9—C33—H33C	109.5
N11—C11—C1	175.8 (2)	H33A—C33—H33C	109.5
C17—C12—C13	121.3 (2)	H33B—C33—H33C	109.5
C17—C12—N3	120.32 (19)	O34—C34—N34	125.3 (2)
C13—C12—N3	118.38 (19)	O34—C34—H34	117.3
C14—C13—C12	119.2 (2)	N34—C34—H34	117.3
C14—C13—H13	120.4	N34—C35—H35A	109.5
C12—C13—H13	120.4	N34—C35—H35B	109.5

C15—C14—C13	120.1 (2)	H35A—C35—H35B	109.5
C15—C14—H14	119.9	N34—C35—H35C	109.5
C13—C14—H14	119.9	H35A—C35—H35C	109.5
C14—C15—C16	120.0 (2)	H35B—C35—H35C	109.5
C14—C15—H15	120.0	N34—C36—H36A	109.5
C16—C15—H15	120.0	N34—C36—H36B	109.5
C17—C16—C15	120.2 (2)	H36A—C36—H36B	109.5
C17—C16—H16	119.9	N34—C36—H36C	109.5
C15—C16—H16	119.9	H36A—C36—H36C	109.5
C12—C17—C16	119.1 (2)	H36B—C36—H36C	109.5
C12—C17—H17	120.4	C2—N2—H2N	112.5 (17)
C16—C17—H17	120.4	C4—N3—C2	124.93 (17)
C23—C18—C19	117.73 (19)	C4—N3—C12	117.45 (17)
C23—C18—C6	119.75 (19)	C2—N3—C12	117.42 (17)
C19—C18—C6	122.41 (18)	C10—N10—H10N	112.8 (17)
C20—C19—C18	120.7 (2)	C34—N34—C35	120.03 (19)
C20—C19—H19	119.7	C34—N34—C36	121.7 (2)
C18—C19—H19	119.7	C35—N34—C36	117.86 (19)
C19—C20—C21	121.7 (2)	C10—O9—C9	116.16 (15)
C19—C20—H20	119.2		

C11—C1—C2—N2	−21.8 (3)	N3—C12—C13—C14	179.8 (2)
C9—C1—C2—N2	−141.3 (2)	C12—C13—C14—C15	−0.5 (3)
C8—C1—C2—N2	99.8 (2)	C13—C14—C15—C16	0.2 (4)
C11—C1—C2—N3	162.27 (17)	C14—C15—C16—C17	−0.2 (3)
C9—C1—C2—N3	42.7 (2)	C13—C12—C17—C16	−0.7 (3)
C8—C1—C2—N3	−76.1 (2)	N3—C12—C17—C16	−179.82 (19)
O4—C4—C5—C9	161.19 (19)	C15—C16—C17—C12	0.4 (3)
N3—C4—C5—C9	−19.4 (3)	C5—C6—C18—C23	−156.70 (18)
O4—C4—C5—C6	−74.4 (2)	C7—C6—C18—C23	83.9 (2)
N3—C4—C5—C6	105.0 (2)	C5—C6—C18—C19	27.2 (3)
C4—C5—C6—C18	128.31 (18)	C7—C6—C18—C19	−92.2 (2)
C9—C5—C6—C18	−105.81 (19)	C23—C18—C19—C20	−3.6 (3)
C4—C5—C6—C7	−109.82 (18)	C6—C18—C19—C20	172.57 (19)
C9—C5—C6—C7	16.1 (2)	C18—C19—C20—C21	−1.2 (3)
C18—C6—C7—C25	−64.0 (2)	C19—C20—C21—C22	5.1 (3)
C5—C6—C7—C25	171.40 (16)	C19—C20—C21—C24	−172.4 (2)
C18—C6—C7—C10	57.3 (2)	C20—C21—C22—C23	−4.2 (3)
C5—C6—C7—C10	−67.34 (19)	C24—C21—C22—C23	173.3 (2)
C18—C6—C7—C8	176.56 (16)	C21—C22—C23—C18	−0.5 (3)
C5—C6—C7—C8	51.9 (2)	C19—C18—C23—C22	4.4 (3)
C25—C7—C8—C26	47.0 (2)	C6—C18—C23—C22	−171.82 (19)
C10—C7—C8—C26	−78.3 (2)	C7—C8—C26—C31	−148.55 (19)
C6—C7—C8—C26	166.10 (16)	C1—C8—C26—C31	87.2 (2)
C25—C7—C8—C1	173.51 (16)	C7—C8—C26—C27	35.4 (3)
C10—C7—C8—C1	48.2 (2)	C1—C8—C26—C27	−88.9 (2)
C6—C7—C8—C1	−67.4 (2)	C31—C26—C27—C28	−0.3 (3)
C11—C1—C8—C26	19.3 (2)	C8—C26—C27—C28	175.78 (19)

C2—C1—C8—C26	−100.43 (19)	C26—C27—C28—C29	−1.0 (3)
C9—C1—C8—C26	139.59 (17)	C27—C28—C29—C30	1.4 (3)
C11—C1—C8—C7	−109.61 (19)	C27—C28—C29—C32	−177.4 (2)
C2—C1—C8—C7	130.67 (17)	C28—C29—C30—C31	−0.6 (3)
C9—C1—C8—C7	10.7 (2)	C32—C29—C30—C31	178.2 (2)
C4—C5—C9—O9	167.19 (16)	C29—C30—C31—C26	−0.7 (3)
C6—C5—C9—O9	43.6 (2)	C27—C26—C31—C30	1.1 (3)
C4—C5—C9—C33	−74.8 (2)	C8—C26—C31—C30	−175.21 (19)
C6—C5—C9—C33	161.62 (17)	O4—C4—N3—C2	175.69 (19)
C4—C5—C9—C1	51.1 (2)	C5—C4—N3—C2	−3.7 (3)
C6—C5—C9—C1	−72.5 (2)	O4—C4—N3—C12	1.0 (3)
C11—C1—C9—O9	59.6 (2)	C5—C4—N3—C12	−178.45 (17)
C2—C1—C9—O9	179.10 (15)	N2—C2—N3—C4	175.9 (2)
C8—C1—C9—O9	−62.54 (19)	C1—C2—N3—C4	−8.5 (3)
C11—C1—C9—C33	−57.5 (2)	N2—C2—N3—C12	−9.4 (3)
C2—C1—C9—C33	62.1 (2)	C1—C2—N3—C12	166.25 (17)
C8—C1—C9—C33	−179.57 (16)	C17—C12—N3—C4	−98.1 (2)
C11—C1—C9—C5	177.32 (16)	C13—C12—N3—C4	82.8 (2)
C2—C1—C9—C5	−63.1 (2)	C17—C12—N3—C2	86.7 (2)
C8—C1—C9—C5	55.2 (2)	C13—C12—N3—C2	−92.4 (2)
C25—C7—C10—N10	−1.0 (3)	O34—C34—N34—C35	5.8 (4)
C8—C7—C10—N10	122.2 (2)	O34—C34—N34—C36	178.1 (2)
C6—C7—C10—N10	−119.4 (2)	N10—C10—O9—C9	−177.47 (19)
C25—C7—C10—O9	176.72 (16)	C7—C10—O9—C9	4.7 (2)
C8—C7—C10—O9	−60.1 (2)	C33—C9—O9—C10	178.80 (16)
C6—C7—C10—O9	58.3 (2)	C5—C9—O9—C10	−59.0 (2)
C17—C12—C13—C14	0.8 (3)	C1—C9—O9—C10	56.6 (2)

Hydrogen-bond geometry (Å, º)

*Cg*7 is the centroid of the C26–C31 benzene ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H6···O34	1.00	2.44	3.297 (3)	143
C8—H8···O34	1.00	2.34	3.241 (3)	149
C13—H13···O34	0.95	2.47	3.373 (3)	159
C27—H27···N10	0.95	2.56	3.432 (3)	152
C30—H30···N11^{i}	0.95	2.61	3.515 (3)	160
C33—H33*C*···O4^{ii}	0.98	2.48	3.447 (3)	170
C35—H35*C*···O34	0.98	2.39	2.787 (3)	104
C24—H24*C*···*Cg*7^{iii}	0.98	2.84	3.715 (2)	148

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