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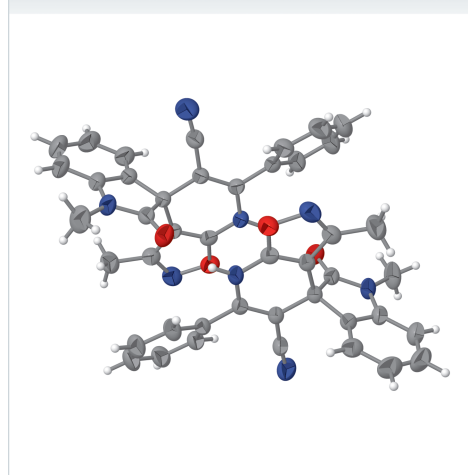
1,3'-Dimethyl-2-oxo-6'-phenyl-7'H-spiro[indoline-3,4'-isoxazolo[5,4-b]pyridine]-5'-carbonitrile

S. Logalakshmi,^{a*} Panneerselvam Yuvaraj,^b Dhruva Jyoti Boruah,^c R. Raja^d and G. Puthilibai^a

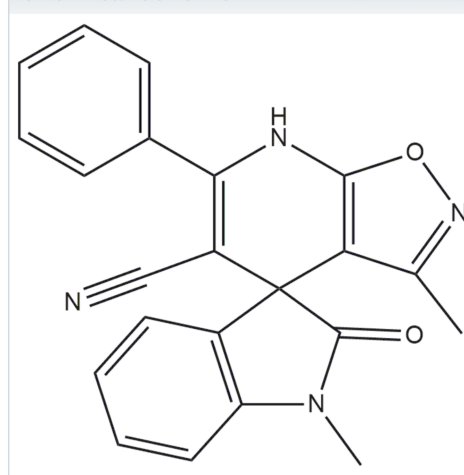
^aDepartment of Chemistry, Sri Sairam Engineering College (Autonomous), Chennai - 600 044, India, ^bChemical Sciences & Technology Division, CSIR-North East Institute of Science & Technology (NEIST), Assam - 785006, India, ^cAcademy of Scientific and Innovative Research (AcSIR), Ghaziabad - 201002, India, and ^dDepartment of Physics, Thiruthangal Nadar College, Chennai - 600 051, India. *Correspondence e-mail: logalakshmi9@gmail.com

The title compound, C₂₂H₁₆N₄O₂, crystallizes in the monoclinic space group *P*2₁/*c* with two independent molecules, *A* and *B*, in the asymmetric unit. The isoxazole ring is inclined to the pyridine ring system, the indoline ring, and the phenyl ring by 8.00 (10), 70.93 (10), 35.89 (12), respectively, ° for molecule *A*, and 4.24 (10), 84.62 (9), 30.02 (11)° for molecule *B*. In the crystal, molecules are linked by C—H···O and C—H···N interactions, forming layers parallel to the (100) plane. In addition π - π interactions with centroid-to-centroid distances of 3.8057 (12) Å and a series of C—H··· π interactions help to consolidate the packing in a three-dimensional architecture within the crystal. Additional electron density was localized in voids (398 Å³ solvent accessible volume) summing up to 92 electrons, which corresponds to approximately 3.5 molecules of ethanol. The given chemical formula and other crystal data do not take into account the solvent.

3D view



Chemical scheme



Structure description

Nitrogen-containing heterocyclic compounds have attracted the attention of many researchers during the decades-long historical development of organic synthesis (Dömling *et al.*, 2000). Many heterocyclic compounds exhibit many biological properties such as anticonvulsant, antitumour, antineoplastic, antiseptic, antiviral, and hypnotic properties, *etc.* In particular, the indole nucleus occurs in a variety of natural products and medicinal agents (de Graaff *et al.*, 2012). Therefore, natural products with a heterocyclic ring structure are attracting considerable attention in the fields of pharmaceuticals and synthetic organic chemistry (Houlihan *et al.*, 1992).

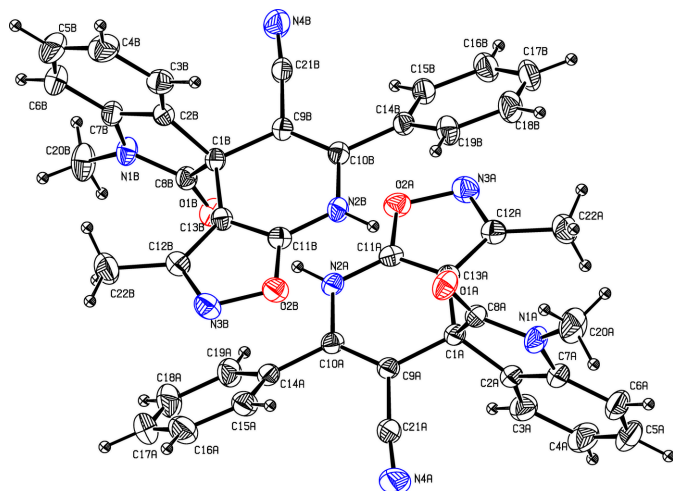


Figure 1
The molecular structures of molecules *A* and *B* in the title compound with displacement ellipsoids drawn at the 30% probability level.

The title compound crystallizes in the monoclinic space group $P2_1/c$ with two molecules (labelled *A* and *B*) in the asymmetric unit (Fig. 1). The molecular structure is characterized by a spiro junction connecting the indoline core with the isoxazolo[5,4-*b*]pyridine ring system. The indoline moiety is substituted at the isatin with a phenyl group and at the 2-position with a keto group, forming a 2-oxindoline derivative. The two molecules have slightly different conformations. Fig. 2 shows a superposition of the two molecules using *PLATON* (Spek *et al.*, 2020) highlighting the differences in their conformations; the root-mean-square deviation is 0.140 Å after inversion. The observed deviation is attributed to the torsional twisting of the phenyl ring with respect to the pyridine ring. For example, the torsion angle between atoms

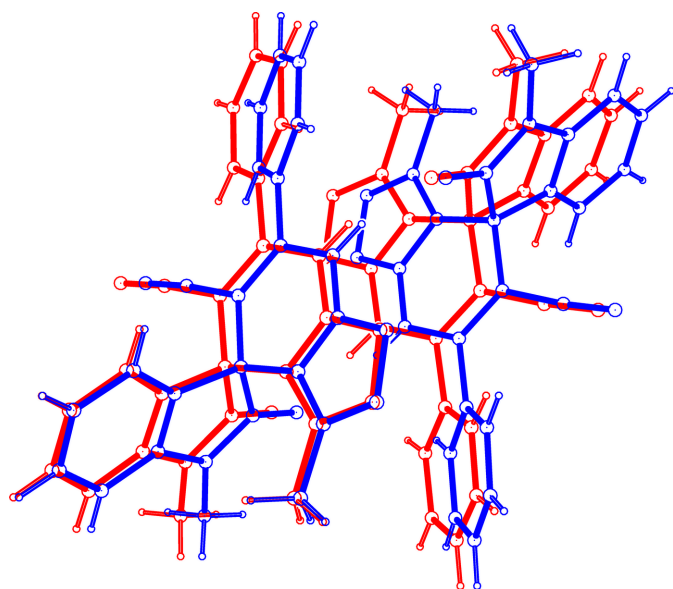


Figure 2
Superposition of molecule *A* (red) and molecule *B* (blue) for the title compound.

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

Cg2 is the centroid of the N1A/C7A/C2A/C1A/C8A ring.

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
N2A—H2A...O1B	0.86	2.09	2.910 (2)	159
N2B—H2B...O1A	0.86	1.92	2.731 (2)	156
C6A—H6A...N4B ⁱ	0.93	2.62	3.299 (3)	130
C6B—H6B...N4A ⁱⁱ	0.93	2.62	3.496 (3)	157
C19A—H19A...O1B ⁱⁱⁱ	0.93	2.50	3.377 (3)	157
C22A—H22B... <i>Cg2</i>	0.96	2.95	3.314 (3)	103

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

N2A—C10A—C14A—C19A is $39.9(2)^\circ$ in molecule *A* and N2B—C10B—C14B—C19B is $-32.1(2)^\circ$ in molecule *B*. The bond lengths C21A—N4A [1.142 (3) Å] and C21B—N4B [1.148 (3) Å] confirm the triple-bond character. In molecule *A*, atoms O1A, C20A and C22A deviate by $-0.081(2)$, $0.107(3)$ and $-0.244(3)$ Å, respectively, from the least-squares plane through the ring to which they are attached (C1A—C2A—C7A—N1A—C8A and C13A—C12A—N3A—O2A—C11A). The deviations for the corresponding atoms in molecule *B* are $0.059(3)$, $-0.076(6)$ and $0.177(3)$ Å, respectively. The pyridine (C11A—N2A—C10A—C9A—C1A—C13A) and phenyl (C14A—C19A) rings subtend a dihedral angle of $41.13(10)^\circ$ in molecule *A* and $33.36(10)^\circ$ in molecule *B*.

In the crystal, molecules are linked by intermolecular N—H...O, C—H...O and C—H...N interactions, forming dimers and layers parallel to the (100) plane (Table 1; Figs. 3 and 4). In addition, π — π [$Cg1 \cdots Cg12 = 3.8057(12)$ Å; *Cg1* and *Cg12* are the centroids of isoxazole O2A—N3A—C12A—C13A—C11A and phenyl C14B—C19B ring, respectively] and C—H... π interactions connect the molecules within the layers that are also connected by van der Waals interactions.

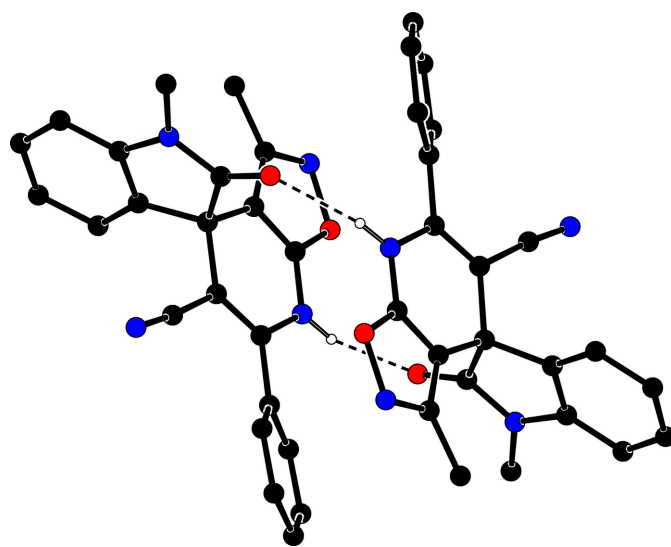


Figure 3
A partial packing diagram for the title compound. N—H...O hydrogen bonds are shown as dashed lines. H atoms not involved in these interactions have been omitted for clarity.

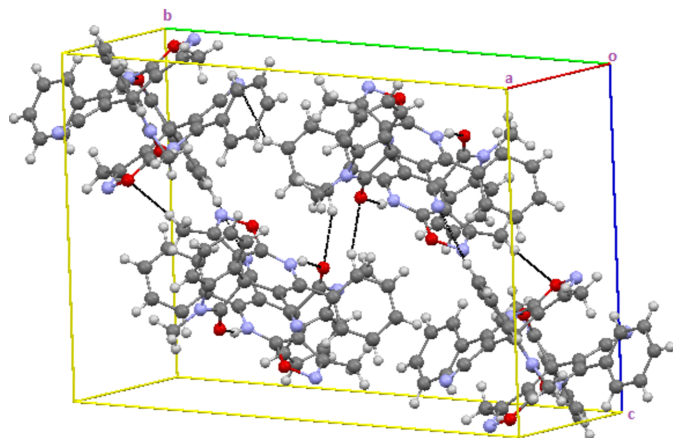


Figure 4
A view of the molecular packing showing the C—H···O and C—H···N interactions.

Synthesis and crystallization

In a 50 ml round-bottom flask, 1*H*-indole-2,3-dione (0.5 mmol) was dissolved in toluene (5 ml) and then 3-oxo-3-phenylpropanenitrile (0.5 mmol) and 5-amino-3-methylisoxazole (0.5 mmol) were added to it. To the stirring reaction mixture was added *p*-toluenesulfonic acid (30 mole %), and stirring was continued under reflux conditions for 10 h at 383 K. The purified compound, obtained by column chromatography, was crystallized from ethanol solution.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Additional electron density was localized in voids (398 Å³ solvent accessible volume) summing up to 92 electrons, which corresponds to approximately 3.5 molecules of ethanol.

Acknowledgements

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Table 2

Experimental details.

Crystal data	
Chemical formula	C ₂₂ H ₁₆ N ₄ O ₂
<i>M_r</i>	368.39
Crystal system, space group	Monoclinic, <i>P</i> 2 ₁ / <i>c</i>
Temperature (K)	294
<i>a</i> , <i>b</i> , <i>c</i> (Å)	13.6520 (2), 19.5065 (3), 15.3599 (3)
β (°)	104.7906 (7)
<i>V</i> (Å ³)	3954.85 (11)
<i>Z</i>	8
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	0.08
Crystal size (mm)	0.28 × 0.25 × 0.16
Data collection	
Diffractometer	Bruker D8 QUEST PHOTON-100
Absorption correction	Multi-scan (<i>SADABS</i> ; Krause <i>et al.</i> , 2015)
<i>T_{min}</i> , <i>T_{max}</i>	0.658, 0.746
No. of measured, independent and observed [<i>I</i> > 2 σ (<i>I</i>)] reflections	34243, 6957, 5203
<i>R_{int}</i>	0.044
(<i>sin</i> θ / λ) _{max} (Å ⁻¹)	0.595
Refinement	
<i>R</i> [<i>F</i> ² > 2 σ (<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.046, 0.132, 1.05
No. of reflections	6957
No. of parameters	509
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}$, $\Delta\rho_{\text{min}}$ (e Å ⁻³)	0.18, -0.23

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*) and *SHELXTL* (Sheldrick, 2008).

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full crystallographic data

IUCrData (2026). **11**, x260232 [https://doi.org/10.1107/S2414314626002324]

1,3'-Dimethyl-2-oxo-6'-phenyl-7'*H*-spiro[indoline-3,4'-isoxazolo[5,4-*b*]pyridine]-5'-carbonitrile

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1,3'-Dimethyl-2-oxo-6'-phenyl-7'*H*-spiro[indoline-3,4'-isoxazolo[5,4-*b*]pyridine]-5'-carbonitrile

Crystal data

C₂₂H₁₆N₄O₂

$M_r = 368.39$

Monoclinic, $P2_1/c$

$a = 13.6520$ (2) Å

$b = 19.5065$ (3) Å

$c = 15.3599$ (3) Å

$\beta = 104.7906$ (7)°

$V = 3954.85$ (11) Å³

$Z = 8$

$F(000) = 1744$

$D_x = 1.237$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 9936 reflections

$\theta = 2.5$ – 30.4 °

$\mu = 0.08$ mm⁻¹

$T = 294$ K

Block, colorless

$0.28 \times 0.25 \times 0.16$ mm

Data collection

Bruker D8 QUEST PHOTON-100
diffractometer

ω and ϕ scans

Absorption correction: multi-scan
(SADABS; Krause *et al.*, 2015)

$T_{\min} = 0.658$, $T_{\max} = 0.746$

34243 measured reflections

6957 independent reflections

5203 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.044$

$\theta_{\max} = 25.0$ °, $\theta_{\min} = 2.5$ °

$h = -16 \rightarrow 16$

$k = -22 \rightarrow 23$

$l = -18 \rightarrow 18$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.046$

$wR(F^2) = 0.132$

$S = 1.05$

6957 reflections

509 parameters

0 restraints

Hydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0521P)^2 + 1.8268P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.18$ e Å⁻³

$\Delta\rho_{\min} = -0.23$ 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. Hydrogen atoms were positioned geometrically (C—H = 0.93–0.98 Å) and allowed to ride on their parent atoms, with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for methyl H and $1.2U_{\text{eq}}(\text{C})$ for other H atoms.

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1A	0.89488 (13)	0.63143 (9)	0.62356 (13)	0.0369 (4)
C2A	0.98261 (14)	0.63155 (10)	0.57954 (14)	0.0429 (5)
C3A	0.99273 (18)	0.60113 (12)	0.50136 (17)	0.0587 (6)
H3A	0.943197	0.571606	0.468940	0.070*
C4A	1.0791 (2)	0.61569 (14)	0.4721 (2)	0.0733 (8)
H4A	1.087295	0.595662	0.419457	0.088*
C5A	1.15200 (19)	0.65924 (15)	0.5200 (2)	0.0767 (8)
H5A	1.208834	0.668357	0.499043	0.092*
C6A	1.14306 (17)	0.68984 (13)	0.59863 (19)	0.0652 (7)
H6A	1.192735	0.719233	0.631116	0.078*
C7A	1.05747 (14)	0.67504 (11)	0.62696 (16)	0.0479 (5)
C8A	0.93893 (13)	0.67726 (10)	0.70769 (14)	0.0398 (5)
C9A	0.86335 (13)	0.56076 (9)	0.65162 (13)	0.0385 (4)
C10A	0.76637 (13)	0.53730 (9)	0.63614 (13)	0.0366 (4)
C11A	0.70945 (13)	0.63465 (10)	0.54961 (13)	0.0370 (4)
C12A	0.78519 (15)	0.72100 (10)	0.50493 (14)	0.0435 (5)
C13A	0.80136 (13)	0.66314 (9)	0.56297 (13)	0.0369 (4)
C14A	0.73617 (13)	0.46977 (10)	0.66480 (14)	0.0399 (5)
C15A	0.77555 (16)	0.44455 (11)	0.75064 (15)	0.0499 (5)
H15A	0.825165	0.469124	0.791455	0.060*
C16A	0.7413 (2)	0.38276 (13)	0.77603 (19)	0.0662 (7)
H16A	0.766967	0.366440	0.834299	0.079*
C17A	0.6697 (2)	0.34550 (13)	0.7155 (2)	0.0730 (8)
H17A	0.647519	0.303735	0.732660	0.088*
C18A	0.63098 (19)	0.36966 (13)	0.6303 (2)	0.0711 (7)
H18A	0.583315	0.343932	0.589193	0.085*
C19A	0.66221 (16)	0.43201 (11)	0.60502 (16)	0.0538 (6)
H19A	0.633635	0.448947	0.547545	0.065*
C20A	1.08696 (18)	0.75127 (14)	0.76617 (19)	0.0746 (8)
H20A	1.080156	0.795770	0.738583	0.112*
H20B	1.157133	0.738346	0.782933	0.112*
H20C	1.061405	0.752560	0.818862	0.112*
C21A	0.94644 (15)	0.51870 (11)	0.69577 (16)	0.0509 (5)
C22A	0.85997 (18)	0.77382 (12)	0.49384 (18)	0.0626 (6)
H22A	0.906826	0.753838	0.463961	0.094*
H22B	0.896233	0.790473	0.551943	0.094*
H22C	0.825004	0.811175	0.458458	0.094*
O1A	0.89919 (10)	0.69017 (8)	0.76840 (10)	0.0520 (4)
O2A	0.63896 (10)	0.66892 (7)	0.48864 (9)	0.0481 (4)
N1A	1.02952 (12)	0.70132 (9)	0.70255 (12)	0.0482 (4)
N2A	0.68608 (11)	0.57551 (8)	0.58637 (11)	0.0409 (4)
H2A	0.624352	0.562432	0.579059	0.049*
N3A	0.69019 (14)	0.72635 (9)	0.45955 (12)	0.0528 (5)
N4A	1.01792 (15)	0.48861 (11)	0.72916 (19)	0.0846 (8)
C1B	0.49623 (13)	0.61809 (9)	0.74448 (12)	0.0344 (4)

C2B	0.41311 (14)	0.62528 (10)	0.79318 (13)	0.0382 (4)
C3B	0.41023 (17)	0.66276 (11)	0.86851 (14)	0.0493 (5)
H3B	0.462583	0.692614	0.894708	0.059*
C4B	0.3270 (2)	0.65488 (14)	0.90445 (18)	0.0664 (7)
H4B	0.323381	0.679566	0.955323	0.080*
C5B	0.2497 (2)	0.61024 (15)	0.86443 (19)	0.0723 (8)
H5B	0.194912	0.605280	0.889489	0.087*
C6B	0.25150 (17)	0.57295 (13)	0.78865 (18)	0.0611 (6)
H6B	0.198866	0.543431	0.762059	0.073*
C7B	0.33438 (14)	0.58113 (10)	0.75380 (14)	0.0431 (5)
C8B	0.44666 (13)	0.56811 (10)	0.66731 (13)	0.0381 (4)
C9B	0.52764 (13)	0.68547 (9)	0.70758 (12)	0.0361 (4)
C10B	0.62397 (13)	0.71009 (9)	0.72305 (12)	0.0350 (4)
C11B	0.68074 (13)	0.61514 (10)	0.81534 (12)	0.0367 (4)
C12B	0.60877 (15)	0.52833 (10)	0.86216 (14)	0.0441 (5)
C13B	0.58972 (14)	0.58611 (9)	0.80438 (12)	0.0356 (4)
C14B	0.65493 (14)	0.77549 (10)	0.68854 (13)	0.0387 (4)
C15B	0.60827 (16)	0.80081 (11)	0.60372 (15)	0.0471 (5)
H15B	0.553062	0.777648	0.567754	0.056*
C16B	0.64272 (19)	0.86005 (12)	0.57189 (17)	0.0589 (6)
H16B	0.610379	0.876388	0.514923	0.071*
C17B	0.7241 (2)	0.89481 (12)	0.62362 (19)	0.0644 (7)
H17B	0.747369	0.934438	0.601835	0.077*
C18B	0.77107 (19)	0.87068 (12)	0.70796 (19)	0.0631 (7)
H18B	0.826506	0.894054	0.743221	0.076*
C19B	0.73663 (17)	0.81194 (11)	0.74084 (16)	0.0516 (5)
H19B	0.768351	0.796623	0.798477	0.062*
C20B	0.29114 (19)	0.49726 (14)	0.62356 (18)	0.0694 (7)
H20D	0.325173	0.478147	0.581661	0.104*
H20E	0.229157	0.518549	0.591115	0.104*
H20F	0.276290	0.461463	0.661141	0.104*
C21B	0.44443 (15)	0.72252 (11)	0.65336 (14)	0.0430 (5)
C22B	0.53722 (19)	0.47476 (13)	0.87759 (19)	0.0695 (7)
H22D	0.512771	0.448528	0.823510	0.104*
H22E	0.481144	0.496265	0.893812	0.104*
H22F	0.571655	0.444962	0.925391	0.104*
O1B	0.48352 (10)	0.54880 (8)	0.60710 (9)	0.0486 (4)
O2B	0.75351 (10)	0.58099 (7)	0.87432 (10)	0.0475 (4)
N1B	0.35605 (12)	0.54822 (9)	0.67930 (11)	0.0455 (4)
N2B	0.70321 (11)	0.67387 (8)	0.77696 (11)	0.0406 (4)
H2B	0.764694	0.687937	0.786014	0.049*
N3B	0.70454 (14)	0.52351 (9)	0.90502 (12)	0.0513 (4)
N4B	0.37283 (14)	0.74794 (11)	0.60951 (15)	0.0655 (6)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1A	0.0285 (9)	0.0354 (10)	0.0453 (11)	-0.0014 (7)	0.0069 (8)	-0.0009 (8)

C2A	0.0338 (10)	0.0389 (11)	0.0565 (13)	0.0007 (8)	0.0126 (9)	0.0001 (10)
C3A	0.0532 (13)	0.0555 (14)	0.0709 (16)	-0.0007 (11)	0.0223 (12)	-0.0109 (12)
C4A	0.0704 (17)	0.0775 (18)	0.0851 (19)	0.0040 (14)	0.0435 (15)	-0.0159 (15)
C5A	0.0525 (14)	0.0835 (19)	0.108 (2)	-0.0050 (14)	0.0451 (15)	-0.0057 (17)
C6A	0.0411 (12)	0.0694 (16)	0.0908 (19)	-0.0110 (11)	0.0271 (12)	-0.0081 (14)
C7A	0.0335 (10)	0.0465 (12)	0.0648 (14)	-0.0018 (9)	0.0148 (10)	0.0005 (11)
C8A	0.0286 (9)	0.0391 (11)	0.0486 (12)	-0.0014 (8)	0.0037 (9)	0.0027 (9)
C9A	0.0301 (9)	0.0346 (10)	0.0482 (12)	-0.0005 (8)	0.0051 (8)	-0.0015 (9)
C10A	0.0317 (9)	0.0364 (10)	0.0402 (11)	-0.0009 (8)	0.0064 (8)	-0.0058 (8)
C11A	0.0333 (9)	0.0390 (11)	0.0369 (10)	0.0035 (8)	0.0057 (8)	-0.0055 (8)
C12A	0.0458 (11)	0.0449 (11)	0.0393 (11)	0.0026 (9)	0.0103 (9)	0.0012 (9)
C13A	0.0343 (10)	0.0362 (10)	0.0397 (11)	0.0012 (8)	0.0085 (8)	-0.0037 (8)
C14A	0.0337 (9)	0.0363 (10)	0.0505 (12)	-0.0008 (8)	0.0122 (9)	-0.0037 (9)
C15A	0.0508 (12)	0.0433 (12)	0.0544 (13)	0.0014 (10)	0.0113 (10)	-0.0011 (10)
C16A	0.0795 (17)	0.0518 (14)	0.0701 (17)	0.0085 (13)	0.0240 (14)	0.0142 (13)
C17A	0.0758 (17)	0.0464 (14)	0.101 (2)	-0.0125 (13)	0.0316 (16)	0.0081 (15)
C18A	0.0645 (15)	0.0531 (15)	0.092 (2)	-0.0251 (12)	0.0138 (14)	-0.0055 (14)
C19A	0.0465 (12)	0.0488 (13)	0.0622 (14)	-0.0123 (10)	0.0065 (10)	-0.0017 (11)
C20A	0.0539 (14)	0.0772 (18)	0.089 (2)	-0.0288 (13)	0.0109 (13)	-0.0246 (15)
C21A	0.0350 (11)	0.0425 (12)	0.0703 (15)	-0.0028 (9)	0.0045 (10)	0.0044 (11)
C22A	0.0606 (14)	0.0569 (14)	0.0689 (16)	-0.0026 (11)	0.0139 (12)	0.0203 (12)
O1A	0.0397 (7)	0.0646 (10)	0.0520 (9)	-0.0105 (7)	0.0122 (7)	-0.0117 (8)
O2A	0.0375 (7)	0.0528 (9)	0.0483 (8)	0.0044 (6)	0.0005 (6)	0.0022 (7)
N1A	0.0334 (8)	0.0510 (10)	0.0588 (11)	-0.0119 (8)	0.0090 (8)	-0.0110 (9)
N2A	0.0258 (7)	0.0408 (9)	0.0531 (10)	-0.0028 (7)	0.0047 (7)	-0.0014 (8)
N3A	0.0536 (11)	0.0528 (11)	0.0486 (11)	0.0038 (9)	0.0071 (9)	0.0089 (9)
N4A	0.0404 (11)	0.0651 (14)	0.134 (2)	0.0083 (10)	-0.0035 (12)	0.0224 (14)
C1B	0.0328 (9)	0.0350 (10)	0.0347 (10)	-0.0049 (8)	0.0076 (8)	-0.0013 (8)
C2B	0.0379 (10)	0.0367 (10)	0.0411 (11)	0.0017 (8)	0.0121 (8)	0.0062 (9)
C3B	0.0533 (12)	0.0483 (12)	0.0469 (12)	0.0046 (10)	0.0139 (10)	-0.0022 (10)
C4B	0.0740 (17)	0.0739 (17)	0.0610 (15)	0.0132 (14)	0.0350 (13)	-0.0020 (13)
C5B	0.0624 (16)	0.088 (2)	0.0810 (19)	0.0044 (14)	0.0445 (15)	0.0079 (16)
C6B	0.0477 (12)	0.0665 (15)	0.0745 (17)	-0.0093 (11)	0.0253 (12)	0.0046 (13)
C7B	0.0377 (10)	0.0453 (11)	0.0474 (12)	-0.0039 (9)	0.0131 (9)	0.0060 (9)
C8B	0.0338 (9)	0.0380 (10)	0.0405 (11)	-0.0040 (8)	0.0060 (8)	0.0019 (9)
C9B	0.0348 (9)	0.0368 (10)	0.0368 (10)	-0.0029 (8)	0.0094 (8)	0.0000 (8)
C10B	0.0376 (10)	0.0338 (10)	0.0343 (10)	-0.0045 (8)	0.0103 (8)	-0.0065 (8)
C11B	0.0354 (10)	0.0366 (10)	0.0352 (10)	0.0002 (8)	0.0036 (8)	-0.0048 (8)
C12B	0.0483 (11)	0.0399 (11)	0.0437 (11)	-0.0004 (9)	0.0114 (9)	0.0000 (9)
C13B	0.0367 (10)	0.0345 (10)	0.0351 (10)	-0.0032 (8)	0.0081 (8)	-0.0027 (8)
C14B	0.0408 (10)	0.0347 (10)	0.0442 (11)	-0.0038 (8)	0.0175 (9)	-0.0043 (9)
C15B	0.0501 (12)	0.0425 (12)	0.0517 (13)	-0.0037 (9)	0.0187 (10)	0.0018 (10)
C16B	0.0731 (15)	0.0489 (13)	0.0605 (15)	-0.0038 (12)	0.0277 (13)	0.0084 (12)
C17B	0.0822 (17)	0.0404 (13)	0.0817 (19)	-0.0144 (12)	0.0416 (15)	0.0012 (13)
C18B	0.0644 (15)	0.0472 (13)	0.0804 (19)	-0.0228 (11)	0.0237 (13)	-0.0157 (13)
C19B	0.0570 (13)	0.0436 (12)	0.0543 (13)	-0.0152 (10)	0.0146 (11)	-0.0066 (10)
C20B	0.0645 (15)	0.0754 (17)	0.0663 (16)	-0.0387 (13)	0.0130 (13)	-0.0155 (14)
C21B	0.0375 (11)	0.0442 (11)	0.0482 (12)	-0.0057 (9)	0.0125 (9)	0.0066 (10)

C22B	0.0673 (15)	0.0582 (15)	0.0818 (18)	-0.0072 (12)	0.0170 (14)	0.0254 (14)
O1B	0.0457 (8)	0.0577 (9)	0.0436 (8)	-0.0068 (7)	0.0134 (7)	-0.0110 (7)
O2B	0.0399 (7)	0.0441 (8)	0.0516 (9)	-0.0004 (6)	-0.0012 (6)	0.0001 (7)
N1B	0.0397 (9)	0.0493 (10)	0.0474 (10)	-0.0159 (8)	0.0111 (8)	-0.0071 (8)
N2B	0.0317 (8)	0.0397 (9)	0.0478 (10)	-0.0088 (7)	0.0055 (7)	-0.0015 (8)
N3B	0.0562 (11)	0.0428 (10)	0.0506 (11)	0.0008 (8)	0.0057 (9)	0.0054 (8)
N4B	0.0436 (10)	0.0741 (14)	0.0755 (14)	0.0012 (10)	0.0092 (10)	0.0245 (12)

Geometric parameters (Å, °)

C1A—C13A	1.507 (3)	C1B—C13B	1.505 (3)
C1A—C2A	1.518 (3)	C1B—C2B	1.517 (3)
C1A—C9A	1.538 (3)	C1B—C9B	1.535 (2)
C1A—C8A	1.560 (3)	C1B—C8B	1.550 (3)
C2A—C3A	1.378 (3)	C2B—C3B	1.378 (3)
C2A—C7A	1.384 (3)	C2B—C7B	1.389 (3)
C3A—C4A	1.394 (3)	C3B—C4B	1.392 (3)
C3A—H3A	0.9300	C3B—H3B	0.9300
C4A—C5A	1.371 (4)	C4B—C5B	1.385 (4)
C4A—H4A	0.9300	C4B—H4B	0.9300
C5A—C6A	1.380 (4)	C5B—C6B	1.378 (4)
C5A—H5A	0.9300	C5B—H5B	0.9300
C6A—C7A	1.377 (3)	C6B—C7B	1.379 (3)
C6A—H6A	0.9300	C6B—H6B	0.9300
C7A—N1A	1.408 (3)	C7B—N1B	1.408 (3)
C8A—O1A	1.219 (2)	C8B—O1B	1.220 (2)
C8A—N1A	1.344 (2)	C8B—N1B	1.353 (2)
C9A—C10A	1.363 (2)	C9B—C10B	1.363 (2)
C9A—C21A	1.424 (3)	C9B—C21B	1.423 (3)
C10A—N2A	1.383 (2)	C10B—N2B	1.377 (2)
C10A—C14A	1.480 (3)	C10B—C14B	1.484 (3)
C11A—O2A	1.338 (2)	C11B—C13B	1.337 (3)
C11A—C13A	1.339 (3)	C11B—O2B	1.339 (2)
C11A—N2A	1.358 (2)	C11B—N2B	1.359 (2)
C12A—N3A	1.310 (3)	C12B—N3B	1.309 (3)
C12A—C13A	1.420 (3)	C12B—C13B	1.417 (3)
C12A—C22A	1.491 (3)	C12B—C22B	1.490 (3)
C14A—C15A	1.381 (3)	C14B—C15B	1.387 (3)
C14A—C19A	1.390 (3)	C14B—C19B	1.392 (3)
C15A—C16A	1.384 (3)	C15B—C16B	1.383 (3)
C15A—H15A	0.9300	C15B—H15B	0.9300
C16A—C17A	1.373 (4)	C16B—C17B	1.369 (3)
C16A—H16A	0.9300	C16B—H16B	0.9300
C17A—C18A	1.364 (4)	C17B—C18B	1.374 (4)
C17A—H17A	0.9300	C17B—H17B	0.9300
C18A—C19A	1.377 (3)	C18B—C19B	1.382 (3)
C18A—H18A	0.9300	C18B—H18B	0.9300
C19A—H19A	0.9300	C19B—H19B	0.9300

C20A—N1A	1.459 (3)	C20B—N1B	1.456 (3)
C20A—H20A	0.9600	C20B—H20D	0.9600
C20A—H20B	0.9600	C20B—H20E	0.9600
C20A—H20C	0.9600	C20B—H20F	0.9600
C21A—N4A	1.142 (3)	C21B—N4B	1.148 (3)
C22A—H22A	0.9600	C22B—H22D	0.9600
C22A—H22B	0.9600	C22B—H22E	0.9600
C22A—H22C	0.9600	C22B—H22F	0.9600
O2A—N3A	1.450 (2)	O2B—N3B	1.445 (2)
N2A—H2A	0.8600	N2B—H2B	0.8600
C13A—C1A—C2A	111.38 (16)	C13B—C1B—C2B	111.18 (15)
C13A—C1A—C9A	106.69 (14)	C13B—C1B—C9B	107.90 (14)
C2A—C1A—C9A	115.80 (15)	C2B—C1B—C9B	114.69 (15)
C13A—C1A—C8A	111.28 (15)	C13B—C1B—C8B	110.07 (15)
C2A—C1A—C8A	100.77 (14)	C2B—C1B—C8B	101.52 (14)
C9A—C1A—C8A	110.96 (16)	C9B—C1B—C8B	111.39 (15)
C3A—C2A—C7A	119.87 (19)	C3B—C2B—C7B	120.65 (18)
C3A—C2A—C1A	130.81 (18)	C3B—C2B—C1B	130.43 (18)
C7A—C2A—C1A	109.09 (17)	C7B—C2B—C1B	108.73 (16)
C2A—C3A—C4A	118.3 (2)	C2B—C3B—C4B	118.4 (2)
C2A—C3A—H3A	120.8	C2B—C3B—H3B	120.8
C4A—C3A—H3A	120.8	C4B—C3B—H3B	120.8
C5A—C4A—C3A	120.7 (2)	C5B—C4B—C3B	120.0 (2)
C5A—C4A—H4A	119.6	C5B—C4B—H4B	120.0
C3A—C4A—H4A	119.6	C3B—C4B—H4B	120.0
C4A—C5A—C6A	121.6 (2)	C6B—C5B—C4B	122.1 (2)
C4A—C5A—H5A	119.2	C6B—C5B—H5B	119.0
C6A—C5A—H5A	119.2	C4B—C5B—H5B	119.0
C7A—C6A—C5A	117.2 (2)	C5B—C6B—C7B	117.4 (2)
C7A—C6A—H6A	121.4	C5B—C6B—H6B	121.3
C5A—C6A—H6A	121.4	C7B—C6B—H6B	121.3
C6A—C7A—C2A	122.3 (2)	C6B—C7B—C2B	121.5 (2)
C6A—C7A—N1A	127.9 (2)	C6B—C7B—N1B	128.8 (2)
C2A—C7A—N1A	109.76 (17)	C2B—C7B—N1B	109.68 (16)
O1A—C8A—N1A	124.67 (19)	O1B—C8B—N1B	125.66 (18)
O1A—C8A—C1A	126.82 (16)	O1B—C8B—C1B	126.14 (16)
N1A—C8A—C1A	108.51 (17)	N1B—C8B—C1B	108.18 (16)
C10A—C9A—C21A	120.67 (18)	C10B—C9B—C21B	120.92 (17)
C10A—C9A—C1A	125.50 (17)	C10B—C9B—C1B	125.84 (17)
C21A—C9A—C1A	113.82 (15)	C21B—C9B—C1B	113.24 (15)
C9A—C10A—N2A	120.86 (17)	C9B—C10B—N2B	119.92 (17)
C9A—C10A—C14A	125.36 (17)	C9B—C10B—C14B	126.23 (17)
N2A—C10A—C14A	113.71 (15)	N2B—C10B—C14B	113.83 (15)
O2A—C11A—C13A	112.23 (17)	C13B—C11B—O2B	112.32 (17)
O2A—C11A—N2A	120.82 (16)	C13B—C11B—N2B	127.46 (17)
C13A—C11A—N2A	126.81 (17)	O2B—C11B—N2B	120.17 (16)
N3A—C12A—C13A	111.80 (18)	N3B—C12B—C13B	111.85 (18)

N3A—C12A—C22A	119.85 (19)	N3B—C12B—C22B	118.75 (19)
C13A—C12A—C22A	128.31 (19)	C13B—C12B—C22B	129.39 (19)
C11A—C13A—C12A	104.13 (17)	C11B—C13B—C12B	104.02 (17)
C11A—C13A—C1A	122.48 (17)	C11B—C13B—C1B	121.16 (17)
C12A—C13A—C1A	133.25 (17)	C12B—C13B—C1B	134.74 (17)
C15A—C14A—C19A	118.81 (19)	C15B—C14B—C19B	117.93 (19)
C15A—C14A—C10A	122.06 (18)	C15B—C14B—C10B	122.51 (17)
C19A—C14A—C10A	119.05 (18)	C19B—C14B—C10B	119.51 (18)
C14A—C15A—C16A	120.1 (2)	C16B—C15B—C14B	120.9 (2)
C14A—C15A—H15A	119.9	C16B—C15B—H15B	119.5
C16A—C15A—H15A	119.9	C14B—C15B—H15B	119.5
C17A—C16A—C15A	120.2 (2)	C17B—C16B—C15B	120.5 (2)
C17A—C16A—H16A	119.9	C17B—C16B—H16B	119.8
C15A—C16A—H16A	119.9	C15B—C16B—H16B	119.8
C18A—C17A—C16A	120.1 (2)	C16B—C17B—C18B	119.5 (2)
C18A—C17A—H17A	120.0	C16B—C17B—H17B	120.3
C16A—C17A—H17A	120.0	C18B—C17B—H17B	120.3
C17A—C18A—C19A	120.3 (2)	C17B—C18B—C19B	120.5 (2)
C17A—C18A—H18A	119.9	C17B—C18B—H18B	119.7
C19A—C18A—H18A	119.9	C19B—C18B—H18B	119.7
C18A—C19A—C14A	120.4 (2)	C18B—C19B—C14B	120.7 (2)
C18A—C19A—H19A	119.8	C18B—C19B—H19B	119.7
C14A—C19A—H19A	119.8	C14B—C19B—H19B	119.7
N1A—C20A—H20A	109.5	N1B—C20B—H20D	109.5
N1A—C20A—H20B	109.5	N1B—C20B—H20E	109.5
H20A—C20A—H20B	109.5	H20D—C20B—H20E	109.5
N1A—C20A—H20C	109.5	N1B—C20B—H20F	109.5
H20A—C20A—H20C	109.5	H20D—C20B—H20F	109.5
H20B—C20A—H20C	109.5	H20E—C20B—H20F	109.5
N4A—C21A—C9A	174.6 (2)	N4B—C21B—C9B	174.7 (2)
C12A—C22A—H22A	109.5	C12B—C22B—H22D	109.5
C12A—C22A—H22B	109.5	C12B—C22B—H22E	109.5
H22A—C22A—H22B	109.5	H22D—C22B—H22E	109.5
C12A—C22A—H22C	109.5	C12B—C22B—H22F	109.5
H22A—C22A—H22C	109.5	H22D—C22B—H22F	109.5
H22B—C22A—H22C	109.5	H22E—C22B—H22F	109.5
C11A—O2A—N3A	106.52 (14)	C11B—O2B—N3B	106.37 (14)
C8A—N1A—C7A	111.62 (17)	C8B—N1B—C7B	111.65 (16)
C8A—N1A—C20A	122.64 (19)	C8B—N1B—C20B	123.79 (18)
C7A—N1A—C20A	125.66 (18)	C7B—N1B—C20B	124.53 (17)
C11A—N2A—C10A	116.78 (15)	C11B—N2B—C10B	117.62 (15)
C11A—N2A—H2A	121.6	C11B—N2B—H2B	121.2
C10A—N2A—H2A	121.6	C10B—N2B—H2B	121.2
C12A—N3A—O2A	105.32 (16)	C12B—N3B—O2B	105.44 (15)
C13A—C1A—C2A—C3A	-61.0 (3)	C13B—C1B—C2B—C3B	62.6 (3)
C9A—C1A—C2A—C3A	61.2 (3)	C9B—C1B—C2B—C3B	-60.1 (3)
C8A—C1A—C2A—C3A	-179.1 (2)	C8B—C1B—C2B—C3B	179.7 (2)

C13A—C1A—C2A—C7A	113.40 (19)	C13B—C1B—C2B—C7B	-112.24 (18)
C9A—C1A—C2A—C7A	-124.47 (18)	C9B—C1B—C2B—C7B	125.01 (17)
C8A—C1A—C2A—C7A	-4.7 (2)	C8B—C1B—C2B—C7B	4.80 (19)
C7A—C2A—C3A—C4A	-0.3 (3)	C7B—C2B—C3B—C4B	0.5 (3)
C1A—C2A—C3A—C4A	173.5 (2)	C1B—C2B—C3B—C4B	-173.9 (2)
C2A—C3A—C4A—C5A	0.0 (4)	C2B—C3B—C4B—C5B	-0.1 (4)
C3A—C4A—C5A—C6A	0.3 (5)	C3B—C4B—C5B—C6B	-0.5 (4)
C4A—C5A—C6A—C7A	-0.2 (4)	C4B—C5B—C6B—C7B	0.6 (4)
C5A—C6A—C7A—C2A	-0.1 (4)	C5B—C6B—C7B—C2B	-0.1 (3)
C5A—C6A—C7A—N1A	-177.7 (2)	C5B—C6B—C7B—N1B	178.2 (2)
C3A—C2A—C7A—C6A	0.4 (3)	C3B—C2B—C7B—C6B	-0.4 (3)
C1A—C2A—C7A—C6A	-174.7 (2)	C1B—C2B—C7B—C6B	175.07 (19)
C3A—C2A—C7A—N1A	178.4 (2)	C3B—C2B—C7B—N1B	-179.00 (18)
C1A—C2A—C7A—N1A	3.3 (2)	C1B—C2B—C7B—N1B	-3.5 (2)
C13A—C1A—C8A—O1A	66.1 (3)	C13B—C1B—C8B—O1B	-65.3 (2)
C2A—C1A—C8A—O1A	-175.7 (2)	C2B—C1B—C8B—O1B	176.82 (19)
C9A—C1A—C8A—O1A	-52.5 (3)	C9B—C1B—C8B—O1B	54.3 (3)
C13A—C1A—C8A—N1A	-113.50 (18)	C13B—C1B—C8B—N1B	113.30 (17)
C2A—C1A—C8A—N1A	4.7 (2)	C2B—C1B—C8B—N1B	-4.54 (19)
C9A—C1A—C8A—N1A	127.86 (17)	C9B—C1B—C8B—N1B	-127.06 (17)
C13A—C1A—C9A—C10A	-9.7 (3)	C13B—C1B—C9B—C10B	2.9 (3)
C2A—C1A—C9A—C10A	-134.3 (2)	C2B—C1B—C9B—C10B	127.39 (19)
C8A—C1A—C9A—C10A	111.7 (2)	C8B—C1B—C9B—C10B	-118.0 (2)
C13A—C1A—C9A—C21A	169.23 (18)	C13B—C1B—C9B—C21B	-176.91 (16)
C2A—C1A—C9A—C21A	44.6 (2)	C2B—C1B—C9B—C21B	-52.4 (2)
C8A—C1A—C9A—C21A	-69.4 (2)	C8B—C1B—C9B—C21B	62.2 (2)
C21A—C9A—C10A—N2A	-174.26 (19)	C21B—C9B—C10B—N2B	178.96 (18)
C1A—C9A—C10A—N2A	4.6 (3)	C1B—C9B—C10B—N2B	-0.8 (3)
C21A—C9A—C10A—C14A	2.4 (3)	C21B—C9B—C10B—C14B	0.5 (3)
C1A—C9A—C10A—C14A	-178.75 (18)	C1B—C9B—C10B—C14B	-179.26 (17)
O2A—C11A—C13A—C12A	0.6 (2)	O2B—C11B—C13B—C12B	-0.2 (2)
N2A—C11A—C13A—C12A	176.20 (18)	N2B—C11B—C13B—C12B	-177.52 (18)
O2A—C11A—C13A—C1A	-175.64 (16)	O2B—C11B—C13B—C1B	176.96 (16)
N2A—C11A—C13A—C1A	0.0 (3)	N2B—C11B—C13B—C1B	-0.3 (3)
N3A—C12A—C13A—C11A	-0.4 (2)	N3B—C12B—C13B—C11B	0.4 (2)
C22A—C12A—C13A—C11A	177.4 (2)	C22B—C12B—C13B—C11B	-178.3 (2)
N3A—C12A—C13A—C1A	175.2 (2)	N3B—C12B—C13B—C1B	-176.3 (2)
C22A—C12A—C13A—C1A	-7.0 (4)	C22B—C12B—C13B—C1B	5.0 (4)
C2A—C1A—C13A—C11A	134.57 (19)	C2B—C1B—C13B—C11B	-128.85 (19)
C9A—C1A—C13A—C11A	7.3 (2)	C9B—C1B—C13B—C11B	-2.3 (2)
C8A—C1A—C13A—C11A	-113.8 (2)	C8B—C1B—C13B—C11B	119.47 (19)
C2A—C1A—C13A—C12A	-40.4 (3)	C2B—C1B—C13B—C12B	47.3 (3)
C9A—C1A—C13A—C12A	-167.6 (2)	C9B—C1B—C13B—C12B	173.9 (2)
C8A—C1A—C13A—C12A	71.2 (3)	C8B—C1B—C13B—C12B	-64.4 (3)
C9A—C10A—C14A—C15A	46.2 (3)	C9B—C10B—C14B—C15B	-36.5 (3)
N2A—C10A—C14A—C15A	-136.90 (19)	N2B—C10B—C14B—C15B	145.03 (19)
C9A—C10A—C14A—C19A	-137.0 (2)	C9B—C10B—C14B—C19B	146.4 (2)
N2A—C10A—C14A—C19A	39.9 (2)	N2B—C10B—C14B—C19B	-32.1 (2)

C19A—C14A—C15A—C16A	-0.1 (3)	C19B—C14B—C15B—C16B	0.7 (3)
C10A—C14A—C15A—C16A	176.66 (19)	C10B—C14B—C15B—C16B	-176.46 (18)
C14A—C15A—C16A—C17A	1.4 (4)	C14B—C15B—C16B—C17B	0.2 (3)
C15A—C16A—C17A—C18A	-0.8 (4)	C15B—C16B—C17B—C18B	-0.5 (4)
C16A—C17A—C18A—C19A	-1.1 (4)	C16B—C17B—C18B—C19B	-0.2 (4)
C17A—C18A—C19A—C14A	2.4 (4)	C17B—C18B—C19B—C14B	1.2 (4)
C15A—C14A—C19A—C18A	-1.8 (3)	C15B—C14B—C19B—C18B	-1.4 (3)
C10A—C14A—C19A—C18A	-178.7 (2)	C10B—C14B—C19B—C18B	175.86 (19)
C13A—C11A—O2A—N3A	-0.5 (2)	C13B—C11B—O2B—N3B	0.0 (2)
N2A—C11A—O2A—N3A	-176.43 (16)	N2B—C11B—O2B—N3B	177.55 (16)
O1A—C8A—N1A—C7A	177.3 (2)	O1B—C8B—N1B—C7B	-178.58 (19)
C1A—C8A—N1A—C7A	-3.1 (2)	C1B—C8B—N1B—C7B	2.8 (2)
O1A—C8A—N1A—C20A	-5.7 (3)	O1B—C8B—N1B—C20B	3.4 (3)
C1A—C8A—N1A—C20A	173.9 (2)	C1B—C8B—N1B—C20B	-175.2 (2)
C6A—C7A—N1A—C8A	177.8 (2)	C6B—C7B—N1B—C8B	-178.0 (2)
C2A—C7A—N1A—C8A	0.0 (3)	C2B—C7B—N1B—C8B	0.4 (2)
C6A—C7A—N1A—C20A	0.9 (4)	C6B—C7B—N1B—C20B	0.0 (4)
C2A—C7A—N1A—C20A	-177.0 (2)	C2B—C7B—N1B—C20B	178.4 (2)
O2A—C11A—N2A—C10A	168.83 (16)	C13B—C11B—N2B—C10B	2.8 (3)
C13A—C11A—N2A—C10A	-6.5 (3)	O2B—C11B—N2B—C10B	-174.33 (16)
C9A—C10A—N2A—C11A	4.0 (3)	C9B—C10B—N2B—C11B	-2.1 (3)
C14A—C10A—N2A—C11A	-173.04 (16)	C14B—C10B—N2B—C11B	176.53 (16)
C13A—C12A—N3A—O2A	0.1 (2)	C13B—C12B—N3B—O2B	-0.3 (2)
C22A—C12A—N3A—O2A	-177.89 (19)	C22B—C12B—N3B—O2B	178.51 (19)
C11A—O2A—N3A—C12A	0.2 (2)	C11B—O2B—N3B—C12B	0.2 (2)

Hydrogen-bond geometry (Å, °)

Cg2 is the centroid of the N1A/C7A/C2A/C1A/C8A ring.

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
N2A—H2A...O1B	0.86	2.09	2.910 (2)	159
N2B—H2B...O1A	0.86	1.92	2.731 (2)	156
C6A—H6A...N4B ⁱ	0.93	2.62	3.299 (3)	130
C6B—H6B...N4A ⁱⁱ	0.93	2.62	3.496 (3)	157
C19A—H19A...O1B ⁱⁱⁱ	0.93	2.50	3.377 (3)	157
C22A—H22B...Cg2	0.96	2.95	3.314 (3)	103

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