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ISSN 2414-3146

tert-Butyl 4-{3-[6-(4-methoxyphenyl)-2-methylpyrimidin-4-yl]quinolin-2-yl}piperazine-1-carboxylate

Sumati Anthal,[a] Vikram. D. Singh,[b] N. R. Desai,[c] D. B. Arunakumar,[c] S. Sreenivasa,[d] Kamni[b] and Rajni Kant[a]*

[a]Department of Physics, University of Jammu, Jammu Tawi 180 006, India, [b]School of Physics, Shri Mata Vaishno Devi University, Katra 182 320, J&K, India, [c]Department of Chemistry, University College of Science, Tumkur University Tumkur 572 103, India, and [d]Department of Studies and Research in Chemistry, Tumkur University, Tumkur 572 103, Karnataka, India. *Correspondence e-mail: rkant.ju@gmail.com

Received 5 February 2018
Accepted 13 March 2018

Edited by A. J. Lough, University of Toronto, Canada

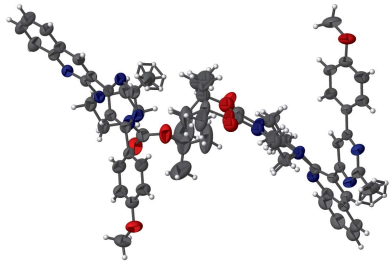
Keywords: crystal structure; quinoline; pyrimidine; direct method; intermolecular hydrogen bonding.

CCDC reference: 1829297

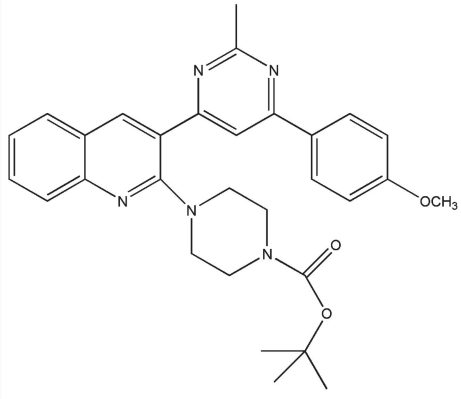
Structural data: full structural data are available from iucrdata.iucr.org

The asymmetric unit of the title compound, $C_{30}H_{33}N_5O_3$, contains two independent molecules, *A* and *B*. In molecule *A*, the *tert*-butyl 4-methylpiperazine-1-carboxylate group was refined as disordered over two sets of sites with an occupancy ratio of 0.821 (4):0.179 (4). The piperazine ring adopts a chair conformation in both molecules. The dihedral angles between the pyrimidine ring and methoxyphenyl ring are 20.27 (14) and 8.72 (11)° for molecules *A* and *B*, respectively. The quinoline ring system makes dihedral angles of 30.68 (11) and 37.76 (10)° with the pyrimidine ring in molecules *A* and *B*, respectively. In the crystal, C—H···O hydrogen bonds link the molecules into chains along [100].

3D view



Chemical scheme



Structure description

Pyrimidine and its derivatives have a diverse array of biological and pharmacological activities including anticonvulsant, antibacterial, antifungal, antiviral and anticancer properties (Jain *et al.*, 2006). An SAR study of the pyrimidine nucleus revealed that substitution at different positions may lead to compounds with a variation in their biological activities (Khanage *et al.*, 2012). Compounds with a pyrimidine ring substituted at the 2 and 4 positions with keto or amino or mixed keto–amino groups have shown anticancer, antiviral, antibacterial and antifungal activity and are used in the treatment of respiratory tract infections and liver disorders. Substitution at the 5 and 6 positions with a heterocyclic ring or a substituted aryl ring leads to anticancer, antiviral, antibacterial and

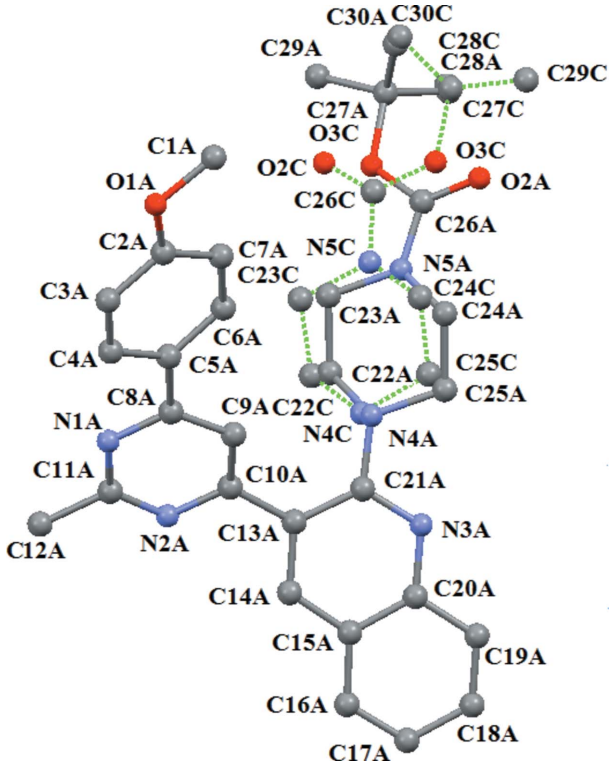


Figure 1
The molecular structure of molecule *A* showing 30% probability displacement ellipsoids. The minor disorder component is shown with green dashed bonds. H atoms are omitted for clarity.

vasodilation activity and such compounds are also used in the treatment of urinary tract infections (Selvam *et al.*, 2012). On the other hand, quinoline derivatives also find importance owing to their wide occurrence in natural products and in biologically active compounds (Markees *et al.*, 1970; Campbell *et al.*, 1988; Kalluraya & Sreenivasa, 1998). As part of our studies in this area, we now describe the synthesis and structure of the title compound.

The asymmetric unit of the title compound comprises two independent molecules, *A* and *B* (Figs. 1 and 2). In both the molecules, the piperazine ring adopts a chair conformation. In

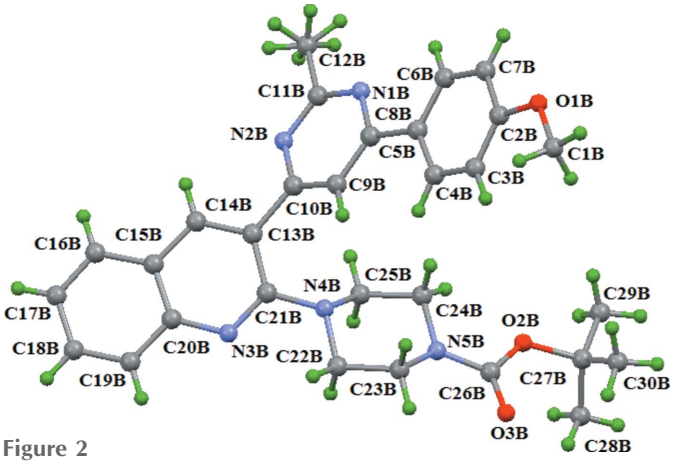


Figure 2
The molecular structure of molecule *B* showing 30% probability displacement ellipsoids.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7*B*—H7*BA*···O2*B*^{i}	0.93	2.40	3.141 (2)	136

Symmetry code: (i) $x+1, y, z$.

the major occupancy component of disordered molecule *A* [0.821 (5) occupancy], the best mirror plane passes through atoms N4*A* and N5*A* and the best twofold rotational axis bisects the N5*A*—C23*A* bond [asymmetry parameter C_s(N4*A*) = 2.53 and C_2(N5*A*—C23*A*) = 1.91] whereas for the minor [0.179 (5)] occupancy component, the best mirror plane passes through atoms C23*C* and C25*C* and the best twofold rotational axis bisects the C22*C*—C23*C* bond [asymmetry parameter C_s(C23*C*) = 1.06 and C_2(C22*C*—C23*C*) = 0.71]. In molecule *B*, the best mirror plane passes through atoms N4*B* and N5*B* and the best twofold rotational axis bisects the N5*B*—C24*B* bond [asymmetry parameter C_s(N4*B*) = 0.54 and C_2(N5*B*—C24*B*) = 5.2] (Duax & Norton, 1975). All bond lengths are in normal ranges and are comparable with those in previously reported related structures (Prasath *et al.*, 2010, 2011; Sharma *et al.*, 2017; Singh *et al.*, 2018). The dihedral angle between the pyrimidine and methoxyphenyl rings is 20.27 (14)° in molecule *A* and 8.72 (11)° in molecule *B* while the pyrimidine ring makes a dihedral angle of 30.68 (11)° in *A* and 37.76 (10)° in *B* with the quinoline ring system. The quinoline units are essentially planar with a maximum deviation of 0.0851 (1) Å for atom C21*A* and 0.0607 (1) Å for C21*B*.

In the crystal, adjacent molecules are linked by C—H···O hydrogen bonds, forming chains along [100] (Table 1 and Fig. 3).

Synthesis and crystallization

2-(4-N-Boc-piperazin-1-yl) quinoline chalcone (1000 mg, 0.00258 mmol), acetamidine hydrochloride (199 mg, 0.002211 mmol) and NaOH (253 mg, 0.00633 mmol) were refluxed for 12 h in ethanol. The progress of the reaction was

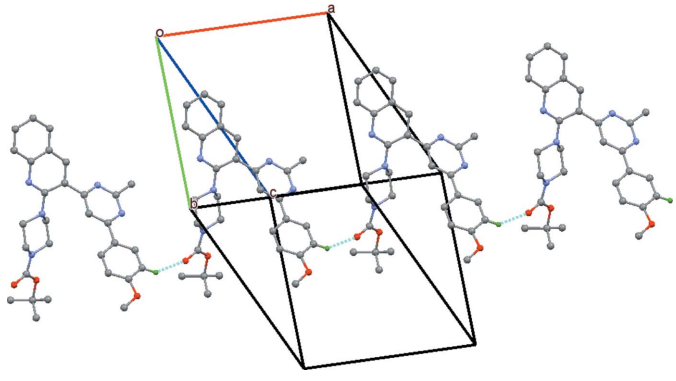


Figure 3
Partial packing plot. Dashed lines indicate the C—H···O intermolecular interactions forming chains along [100]. H atoms not involved in these interactions have been omitted for clarity.

monitored by thin layer chromatography. After the completion of reaction, the reaction mixture was poured into water and extracted with ethyl acetate. The organic layer was washed with water, dried and concentrated under vacuum using a rotary evaporator to obtain a solid that was purified by column chromatography using 60–120 mesh silica gel. Crystals of the title compound were obtained by recrystallization from ethyl acetate solution.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Disorder was modeled for the *tert*-butyl 4-methyl piperazine-1-carboxylate group in molecule *A* with an occupancy ratio of 0.821 (4):0.179 (4). In addition, the methyl H atoms attached to C12*A* and C12*B* are also disordered with occupancy ratios of 0.68 (4):0.32 (4) and 0.53 (4):0.47 (4), respectively.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{30}H_{33}N_5O_3$
M_r	511.61
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	293
a, b, c (Å)	11.0894 (6), 12.6875 (6), 20.8953 (9)
α, β, γ (°)	83.663 (4), 75.335 (4), 86.259 (4)
V (Å^3)	2824.6 (2)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.08
Crystal size (mm)	0.30 × 0.20 × 0.20
Data collection	
Diffractometer	Oxford Diffraction Xcalibur Sapphire3
Absorption correction	Multi-scan (*CrysAlis RED*; Oxford Diffraction, 2010)
T_{min}, T_{max}	0.869, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	19560, 9886, 5244
R_{int}	0.042
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.595
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.065, 0.181, 1.03
No. of reflections	9886
No. of parameters	751
No. of restraints	32
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.27, −0.21

Computer programs: *CrysAlis PRO* (Oxford Diffraction, 2010), *SHELXL97* (Sheldrick, 2008), *SHELXL2016* (Sheldrick, 2015), *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2009).

Funding information

Funding for this research was provided by: Indian Council of Medical Research (grant No. BIC/12(14)/2012 to RK); Department of Science and Technology (grant No. EMR/2014/000467 to RK; award No. SR/S2/CMP-47/2003). RK also acknowledges the Department of Science & Technology for a single-crystal X-ray diffractometer sanctioned as a National Facility under project No. SR/S2/CMP-47/2003.

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full crystallographic data

IUCrData (2018). **3**, x180427 [https://doi.org/10.1107/S2414314618004273]

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Crystal data

$C_{30}H_{33}N_5O_3$
M_r = 511.61
Triclinic, $P\overline{1}$
a = 11.0894 (6) Å
b = 12.6875 (6) Å
c = 20.8953 (9) Å
α = 83.663 (4)°
β = 75.335 (4)°
γ = 86.259 (4)°
V = 2824.6 (2) Å^3
Z = 4
$F(000)$ = 1088
D_x = 1.203 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 4885 reflections
θ = 3.8–26.6°
μ = 0.08 mm^{-1}
T = 293 K
Block, white
0.30 × 0.20 × 0.20 mm

Data collection

Oxford Diffraction Xcalibur Sapphire3 diffractometer
Radiation source: fine-focus sealed tube
Detector resolution: 6.1049 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlis RED; Oxford Diffraction, 2010)
T_{min} = 0.869, T_{max} = 1.000
19560 measured reflections
9886 independent reflections
5244 reflections with $I > 2\sigma(I)$
R_{int} = 0.042
θ_{max} = 25.0°, θ_{min} = 3.6°
h = −13→13
k = −15→15
l = −24→24

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.065
$wR(F^2)$ = 0.181
S = 1.03
9886 reflections
751 parameters
32 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.056P)^2 + 0.4039P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}
Extinction correction: SHELXL2016 (Sheldrick, 2015), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0055 (7)

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. All H atoms were positioned geometrically and were treated as riding on their parent C atoms, with C—H distances of 0.93–0.97 Å; and with U_{iso}(H) = 1.2Ueq(C), except for the methyl groups where U_{iso}(H) = 1.5Ueq(C).

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
O1A	0.4112 (2)	0.24904 (15)	0.89015 (12)	0.0782 (7)	
N1A	0.4291 (2)	0.74137 (18)	0.90707 (12)	0.0547 (7)	
N2A	0.3208 (2)	0.90807 (18)	0.89406 (12)	0.0549 (7)	
N3A	−0.0740 (2)	0.95687 (18)	0.83629 (12)	0.0535 (7)	
C1A	0.3435 (4)	0.1902 (2)	0.8577 (2)	0.0910 (13)	
H1AA	0.364378	0.115925	0.864713	0.137*	
H1AB	0.364741	0.212412	0.810897	0.137*	
H1AC	0.255635	0.202571	0.875508	0.137*	
C2A	0.3901 (3)	0.3566 (2)	0.88660 (16)	0.0557 (8)	
C3A	0.4511 (3)	0.4105 (2)	0.92207 (17)	0.0631 (9)	
H3AA	0.503422	0.373218	0.945828	0.076*	
C4A	0.4352 (3)	0.5183 (2)	0.92263 (16)	0.0577 (8)	
H4AA	0.477179	0.553336	0.946796	0.069*	
C5A	0.3575 (3)	0.5764 (2)	0.88772 (13)	0.0439 (7)	
C6A	0.2974 (3)	0.5202 (2)	0.85269 (15)	0.0553 (8)	
H6AA	0.244421	0.556792	0.829052	0.066*	
C7A	0.3135 (3)	0.4115 (2)	0.85170 (16)	0.0607 (9)	
H7AA	0.272351	0.375925	0.827392	0.073*	
C8A	0.3410 (3)	0.6926 (2)	0.88887 (13)	0.0441 (7)	
C9A	0.2394 (3)	0.7501 (2)	0.87395 (13)	0.0461 (7)	
H9AA	0.177416	0.716377	0.862080	0.055*	
C10A	0.2319 (3)	0.8586 (2)	0.87707 (13)	0.0447 (7)	
C11A	0.4142 (3)	0.8467 (2)	0.90806 (16)	0.0573 (8)	
C12A	0.5128 (3)	0.9007 (3)	0.9286 (2)	0.0883 (12)	
H12D	0.523039	0.866999	0.970447	0.132*	0.68 (4)
H12E	0.488240	0.974079	0.932971	0.132*	0.68 (4)
H12F	0.590317	0.895735	0.895541	0.132*	0.68 (4)
H12X	0.544692	0.957543	0.895526	0.132*	0.32 (4)
H12Y	0.579490	0.850463	0.933001	0.132*	0.32 (4)
H12Z	0.477414	0.928807	0.970432	0.132*	0.32 (4)
C13A	0.1206 (3)	0.9268 (2)	0.86981 (14)	0.0453 (7)	
C14A	0.0897 (3)	1.0104 (2)	0.90780 (14)	0.0514 (8)	
H14B	0.144325	1.027588	0.931943	0.062*	
C15A	−0.0226 (3)	1.0711 (2)	0.91138 (14)	0.0517 (8)	
C16A	−0.0554 (3)	1.1607 (2)	0.94699 (15)	0.0657 (9)	
H16B	−0.000588	1.182985	0.969415	0.079*	
C17A	−0.1658 (4)	1.2153 (3)	0.94927 (17)	0.0763 (11)	

H17B	−0.185662	1.275867	0.971721	0.092*	
C18A	−0.2483 (4)	1.1787 (3)	0.91735 (18)	0.0811 (12)	
H18B	−0.325076	1.214441	0.919940	0.097*	
C19A	−0.2206 (3)	1.0926 (3)	0.88262 (17)	0.0693 (10)	
H19B	−0.278427	1.070025	0.862175	0.083*	
C20A	−0.1046 (3)	1.0368 (2)	0.87717 (15)	0.0534 (8)	
C21A	0.0360 (3)	0.9066 (2)	0.83122 (14)	0.0471 (7)	
N4A	0.0650 (6)	0.8296 (5)	0.7862 (3)	0.046 (2)	0.821 (4)
N5A	0.1156 (4)	0.7165 (3)	0.67279 (16)	0.0595 (10)	0.821 (4)
C22A	0.1768 (6)	0.8494 (5)	0.7325 (3)	0.0569 (17)	0.821 (4)
H22A	0.243242	0.869194	0.750750	0.068*	0.821 (4)
H22B	0.159489	0.908089	0.701780	0.068*	0.821 (4)
C23A	0.2187 (5)	0.7528 (4)	0.6955 (2)	0.0584 (12)	0.821 (4)
H23A	0.288056	0.769940	0.657650	0.070*	0.821 (4)
H23B	0.246730	0.696709	0.724492	0.070*	0.821 (4)
C24A	0.0010 (5)	0.7023 (3)	0.7245 (2)	0.0648 (12)	0.821 (4)
H24A	0.012995	0.643983	0.756743	0.078*	0.821 (4)
H24B	−0.064906	0.684583	0.705132	0.078*	0.821 (4)
C25A	−0.0367 (5)	0.8018 (4)	0.7589 (3)	0.0580 (14)	0.821 (4)
H25A	−0.054339	0.859274	0.727514	0.070*	0.821 (4)
H25B	−0.111648	0.790413	0.794376	0.070*	0.821 (4)
O2A	0.0461 (3)	0.6256 (2)	0.60292 (15)	0.0806 (10)	0.821 (4)
O3A	0.2454 (3)	0.6779 (3)	0.57806 (16)	0.0736 (10)	0.821 (4)
C26A	0.1296 (4)	0.6692 (3)	0.6160 (2)	0.0618 (12)	0.821 (4)
C27A	0.2787 (4)	0.6395 (4)	0.51153 (19)	0.0716 (13)	0.821 (4)
C28A	0.1984 (12)	0.6966 (7)	0.4686 (3)	0.115 (5)	0.821 (4)
H28D	0.112601	0.680592	0.487811	0.173*	0.821 (4)
H28E	0.224041	0.673604	0.424767	0.173*	0.821 (4)
H28F	0.207761	0.771734	0.466098	0.173*	0.821 (4)
C29A	0.4124 (4)	0.6716 (4)	0.4865 (2)	0.1048 (19)	0.821 (4)
H29D	0.460597	0.638089	0.515867	0.157*	0.821 (4)
H29E	0.415776	0.747231	0.484935	0.157*	0.821 (4)
H29F	0.445958	0.649747	0.442710	0.157*	0.821 (4)
C30A	0.2686 (11)	0.5201 (6)	0.5179 (5)	0.122 (6)	0.821 (4)
H30D	0.308103	0.488397	0.551669	0.182*	0.821 (4)
H30E	0.308971	0.493401	0.476254	0.182*	0.821 (4)
H30F	0.182220	0.502811	0.529939	0.182*	0.821 (4)
N4C	0.085 (2)	0.836 (2)	0.7815 (14)	0.047 (12)*	0.179 (4)
N5C	0.1755 (15)	0.7272 (14)	0.6637 (7)	0.060 (6)*	0.179 (4)
C22C	0.206 (2)	0.8579 (18)	0.7344 (14)	0.031 (6)*	0.179 (4)
H22E	0.262662	0.880194	0.758237	0.037*	0.179 (4)
H22F	0.194262	0.915838	0.701871	0.037*	0.179 (4)
C23C	0.2630 (15)	0.763 (2)	0.6988 (11)	0.072 (10)*	0.179 (4)
H23E	0.340864	0.781375	0.667239	0.087*	0.179 (4)
H23F	0.280618	0.705894	0.730595	0.087*	0.179 (4)
C24C	0.0558 (16)	0.7045 (16)	0.7084 (10)	0.058 (8)*	0.179 (4)
H24E	0.065108	0.644200	0.739854	0.070*	0.179 (4)
H24F	−0.000913	0.685885	0.683268	0.070*	0.179 (4)

C25C	0.0015 (17)	0.7984 (18)	0.7456 (13)	0.050 (8)*	0.179 (4)
H25E	−0.017292	0.855714	0.714419	0.060*	0.179 (4)
H25F	−0.076294	0.779032	0.777063	0.060*	0.179 (4)
O2C	0.3282 (13)	0.6920 (11)	0.5751 (7)	0.073 (5)*	0.179 (4)
O3C	0.1338 (15)	0.6351 (13)	0.5861 (7)	0.083 (6)*	0.179 (4)
C26C	0.2201 (14)	0.6809 (16)	0.6060 (7)	0.046 (6)*	0.179 (4)
C27C	0.1653 (14)	0.5955 (12)	0.5196 (7)	0.070 (6)*	0.179 (4)
C28C	0.204 (4)	0.6879 (19)	0.4671 (11)	0.065 (13)*	0.179 (4)
H28A	0.224656	0.662758	0.423825	0.098*	0.179 (4)
H28B	0.136505	0.739899	0.470207	0.098*	0.179 (4)
H28C	0.275499	0.719316	0.474140	0.098*	0.179 (4)
C29C	0.0406 (14)	0.5576 (13)	0.5176 (9)	0.076 (6)*	0.179 (4)
H29A	0.047717	0.529127	0.476050	0.114*	0.179 (4)
H29B	0.013994	0.503444	0.553492	0.114*	0.179 (4)
H29C	−0.019517	0.616014	0.522018	0.114*	0.179 (4)
C30C	0.264 (3)	0.507 (2)	0.5163 (17)	0.10 (2)*	0.179 (4)
H30A	0.284381	0.482174	0.473014	0.145*	0.179 (4)
H30B	0.337996	0.533877	0.524238	0.145*	0.179 (4)
H30C	0.234172	0.450245	0.549386	0.145*	0.179 (4)
O1B	0.4659 (2)	1.16589 (17)	0.28836 (13)	0.0853 (8)	
N1B	0.4623 (2)	0.66522 (19)	0.30835 (12)	0.0557 (7)	
N2B	0.3734 (2)	0.52099 (18)	0.27451 (12)	0.0551 (7)	
N3B	0.0359 (2)	0.55788 (18)	0.16688 (12)	0.0520 (6)	
N4B	0.0356 (2)	0.66254 (17)	0.25152 (11)	0.0498 (6)	
N5B	−0.1124 (2)	0.7906 (2)	0.34538 (12)	0.0630 (8)	
C1B	0.3905 (4)	1.2467 (3)	0.26348 (19)	0.0943 (13)	
H1BA	0.422597	1.314778	0.264531	0.141*	
H1BB	0.306494	1.243604	0.290543	0.141*	
H1BC	0.391224	1.236430	0.218548	0.141*	
C2B	0.4366 (3)	1.0626 (2)	0.28821 (16)	0.0606 (9)	
C3B	0.3370 (3)	1.0326 (2)	0.26817 (17)	0.0663 (9)	
H3BA	0.282413	1.083486	0.254246	0.080*	
C4B	0.3181 (3)	0.9249 (2)	0.26880 (16)	0.0619 (9)	
H4BA	0.249447	0.904575	0.255800	0.074*	
C5B	0.3986 (3)	0.8478 (2)	0.28824 (14)	0.0488 (7)	
C6B	0.4954 (3)	0.8812 (2)	0.31091 (15)	0.0598 (9)	
H6BA	0.548875	0.830766	0.326207	0.072*	
C7B	0.5143 (3)	0.9874 (2)	0.31135 (16)	0.0647 (9)	
H7BA	0.579421	1.008000	0.327225	0.078*	
C8B	0.3852 (3)	0.7341 (2)	0.28273 (14)	0.0471 (7)	
C9B	0.3023 (3)	0.6982 (2)	0.25148 (14)	0.0506 (8)	
H9BA	0.250663	0.745740	0.232552	0.061*	
C10B	0.2974 (3)	0.5898 (2)	0.24882 (13)	0.0468 (7)	
C11B	0.4525 (3)	0.5623 (2)	0.30273 (15)	0.0577 (9)	
C12B	0.5392 (4)	0.4855 (3)	0.33093 (18)	0.0829 (12)	
H12A	0.494706	0.424178	0.353327	0.124*	0.53 (4)
H12B	0.571196	0.519033	0.361898	0.124*	0.53 (4)
H12C	0.607200	0.464357	0.295566	0.124*	0.53 (4)

H12H	0.620695	0.514201	0.320534	0.124*	0.47 (4)
H12I	0.544205	0.419346	0.311963	0.124*	0.47 (4)
H12J	0.508201	0.474022	0.378295	0.124*	0.47 (4)
C13B	0.2175 (3)	0.5448 (2)	0.21209 (14)	0.0460 (7)	
C14B	0.2663 (3)	0.4644 (2)	0.17423 (14)	0.0513 (8)	
H14A	0.342992	0.432813	0.177178	0.062*	
C15B	0.2034 (3)	0.4276 (2)	0.13054 (15)	0.0507 (8)	
C16B	0.2510 (3)	0.3443 (2)	0.09124 (16)	0.0642 (9)	
H16A	0.326080	0.309344	0.094095	0.077*	
C17B	0.1869 (4)	0.3149 (3)	0.04889 (18)	0.0759 (10)	
H17A	0.217222	0.258515	0.023653	0.091*	
C18B	0.0765 (4)	0.3686 (3)	0.04325 (18)	0.0782 (11)	
H18A	0.034490	0.348840	0.013448	0.094*	
C19B	0.0286 (3)	0.4503 (3)	0.08085 (16)	0.0684 (9)	
H19A	−0.045362	0.485812	0.076405	0.082*	
C20B	0.0911 (3)	0.4806 (2)	0.12621 (15)	0.0505 (8)	
C21B	0.0952 (3)	0.5863 (2)	0.20887 (14)	0.0459 (7)	
C22B	−0.0774 (3)	0.7163 (2)	0.23884 (15)	0.0597 (9)	
H22C	−0.146901	0.669642	0.254401	0.072*	
H22D	−0.066387	0.734848	0.191477	0.072*	
C23B	−0.1044 (3)	0.8159 (2)	0.27487 (15)	0.0661 (10)	
H23C	−0.038772	0.865391	0.255923	0.079*	
H23D	−0.182533	0.849538	0.269037	0.079*	
C24B	−0.0071 (3)	0.7270 (3)	0.36064 (16)	0.0706 (10)	
H24C	−0.025227	0.704896	0.407932	0.085*	
H24D	0.066415	0.769326	0.349080	0.085*	
C25B	0.0178 (3)	0.6312 (2)	0.32272 (14)	0.0609 (9)	
H25C	0.091885	0.592583	0.330594	0.073*	
H25D	−0.051874	0.584688	0.338109	0.073*	
O2B	−0.2597 (2)	0.9194 (2)	0.37400 (12)	0.0920 (9)	
O3B	−0.1626 (2)	0.8354 (2)	0.44866 (12)	0.0929 (9)	
C26B	−0.1844 (3)	0.8539 (3)	0.38876 (17)	0.0651 (9)	
C27B	−0.2333 (5)	0.8896 (4)	0.5058 (2)	0.0995 (14)	
C28B	−0.3655 (5)	0.8573 (5)	0.5203 (3)	0.181 (3)	
H28G	−0.401764	0.886628	0.484821	0.271*	
H28H	−0.411978	0.883339	0.561224	0.271*	
H28I	−0.367602	0.781332	0.524297	0.271*	
C29B	−0.1713 (6)	0.8443 (5)	0.5595 (2)	0.182 (3)	
H29G	−0.082931	0.853015	0.544378	0.274*	
H29H	−0.187609	0.770219	0.569941	0.274*	
H29I	−0.203714	0.880877	0.598506	0.274*	
C30B	−0.2271 (7)	1.0048 (4)	0.4932 (3)	0.186 (3)	
H30G	−0.276743	1.030462	0.462799	0.280*	
H30H	−0.142085	1.023623	0.474388	0.280*	
H30I	−0.258472	1.036247	0.534293	0.280*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1A	0.0893 (18)	0.0390 (12)	0.108 (2)	0.0004 (12)	−0.0272 (16)	−0.0079 (12)
N1A	0.0546 (16)	0.0462 (14)	0.0688 (17)	−0.0004 (12)	−0.0213 (14)	−0.0169 (12)
N2A	0.0581 (16)	0.0428 (14)	0.0682 (18)	−0.0056 (12)	−0.0198 (14)	−0.0126 (12)
N3A	0.0581 (17)	0.0504 (14)	0.0517 (16)	0.0005 (13)	−0.0136 (13)	−0.0055 (12)
C1A	0.101 (3)	0.048 (2)	0.125 (4)	−0.014 (2)	−0.020 (3)	−0.023 (2)
C2A	0.059 (2)	0.0412 (18)	0.065 (2)	−0.0049 (15)	−0.0103 (17)	−0.0049 (15)
C3A	0.063 (2)	0.0474 (18)	0.085 (2)	0.0040 (16)	−0.0331 (19)	−0.0003 (17)
C4A	0.060 (2)	0.0477 (18)	0.072 (2)	−0.0038 (15)	−0.0272 (18)	−0.0056 (16)
C5A	0.0491 (18)	0.0383 (15)	0.0447 (17)	−0.0046 (13)	−0.0109 (14)	−0.0051 (13)
C6A	0.064 (2)	0.0456 (17)	0.062 (2)	0.0003 (15)	−0.0264 (17)	−0.0083 (15)
C7A	0.079 (2)	0.0421 (17)	0.068 (2)	−0.0072 (16)	−0.0286 (19)	−0.0107 (15)
C8A	0.0508 (18)	0.0411 (16)	0.0408 (16)	−0.0022 (14)	−0.0095 (14)	−0.0093 (12)
C9A	0.0554 (19)	0.0400 (16)	0.0481 (17)	−0.0066 (14)	−0.0209 (15)	−0.0056 (13)
C10A	0.0523 (18)	0.0391 (16)	0.0438 (17)	−0.0012 (14)	−0.0125 (15)	−0.0070 (13)
C11A	0.057 (2)	0.0511 (19)	0.070 (2)	−0.0077 (16)	−0.0217 (18)	−0.0173 (16)
C12A	0.076 (3)	0.063 (2)	0.142 (4)	−0.0108 (19)	−0.044 (3)	−0.032 (2)
C13A	0.0521 (18)	0.0370 (15)	0.0469 (17)	−0.0064 (13)	−0.0117 (15)	−0.0024 (13)
C14A	0.060 (2)	0.0443 (16)	0.0505 (18)	−0.0061 (15)	−0.0131 (16)	−0.0057 (14)
C15A	0.063 (2)	0.0421 (16)	0.0436 (18)	0.0016 (15)	−0.0038 (16)	−0.0019 (13)
C16A	0.087 (3)	0.0550 (19)	0.051 (2)	0.0082 (18)	−0.0082 (19)	−0.0168 (15)
C17A	0.095 (3)	0.066 (2)	0.058 (2)	0.019 (2)	−0.003 (2)	−0.0138 (17)
C18A	0.083 (3)	0.080 (3)	0.068 (3)	0.028 (2)	−0.001 (2)	−0.010 (2)
C19A	0.063 (2)	0.075 (2)	0.064 (2)	0.0113 (18)	−0.0084 (19)	−0.0092 (18)
C20A	0.057 (2)	0.0494 (18)	0.0446 (18)	0.0043 (15)	−0.0003 (16)	0.0020 (14)
C21A	0.0544 (19)	0.0398 (16)	0.0439 (17)	−0.0049 (14)	−0.0067 (15)	−0.0009 (13)
N4A	0.049 (3)	0.047 (3)	0.044 (3)	−0.007 (2)	−0.0084 (18)	−0.0108 (17)
N5A	0.061 (3)	0.071 (2)	0.046 (2)	−0.012 (2)	−0.004 (2)	−0.0205 (17)
C22A	0.059 (4)	0.062 (3)	0.053 (3)	−0.008 (3)	−0.014 (3)	−0.0139 (19)
C23A	0.056 (3)	0.074 (3)	0.045 (3)	−0.001 (3)	−0.008 (2)	−0.016 (2)
C24A	0.065 (3)	0.064 (3)	0.066 (3)	−0.015 (2)	−0.007 (3)	−0.021 (2)
C25A	0.050 (3)	0.066 (3)	0.059 (3)	−0.007 (2)	−0.009 (3)	−0.017 (2)
O2A	0.088 (3)	0.092 (2)	0.068 (2)	−0.0160 (19)	−0.0164 (19)	−0.0331 (16)
O3A	0.073 (3)	0.101 (2)	0.047 (2)	−0.0036 (19)	−0.0081 (19)	−0.0239 (18)
C26A	0.066 (3)	0.059 (3)	0.062 (3)	−0.006 (2)	−0.017 (3)	−0.010 (2)
C27A	0.076 (3)	0.100 (3)	0.038 (2)	0.011 (3)	−0.011 (2)	−0.021 (2)
C28A	0.115 (7)	0.174 (9)	0.064 (4)	0.007 (5)	−0.044 (4)	−0.002 (4)
C29A	0.092 (4)	0.163 (5)	0.057 (3)	0.006 (4)	−0.005 (3)	−0.039 (3)
C30A	0.159 (9)	0.108 (7)	0.103 (7)	0.031 (4)	−0.031 (4)	−0.061 (5)
O1B	0.108 (2)	0.0496 (14)	0.108 (2)	−0.0091 (13)	−0.0438 (17)	−0.0097 (13)
N1B	0.0653 (17)	0.0537 (15)	0.0557 (16)	0.0090 (13)	−0.0282 (14)	−0.0135 (12)
N2B	0.0672 (18)	0.0518 (15)	0.0516 (15)	0.0078 (13)	−0.0257 (14)	−0.0075 (12)
N3B	0.0561 (16)	0.0524 (14)	0.0489 (15)	−0.0057 (12)	−0.0149 (13)	−0.0043 (12)
N4B	0.0564 (16)	0.0491 (14)	0.0442 (14)	0.0047 (12)	−0.0156 (13)	−0.0025 (11)
N5B	0.0701 (18)	0.0679 (17)	0.0520 (17)	0.0253 (14)	−0.0206 (15)	−0.0134 (13)
C1B	0.130 (4)	0.049 (2)	0.106 (3)	0.004 (2)	−0.039 (3)	0.002 (2)

C2B	0.069 (2)	0.050 (2)	0.065 (2)	−0.0040 (17)	−0.0184 (19)	−0.0080 (16)
C3B	0.073 (2)	0.053 (2)	0.078 (2)	0.0089 (17)	−0.029 (2)	−0.0076 (17)
C4B	0.063 (2)	0.059 (2)	0.072 (2)	0.0022 (17)	−0.0307 (18)	−0.0136 (16)
C5B	0.0519 (19)	0.0482 (17)	0.0494 (18)	0.0014 (14)	−0.0178 (15)	−0.0083 (14)
C6B	0.060 (2)	0.058 (2)	0.065 (2)	0.0051 (16)	−0.0235 (18)	−0.0092 (16)
C7B	0.067 (2)	0.054 (2)	0.081 (2)	−0.0037 (17)	−0.033 (2)	−0.0084 (17)
C8B	0.0467 (18)	0.0489 (17)	0.0456 (17)	0.0016 (14)	−0.0130 (15)	−0.0030 (14)
C9B	0.0528 (19)	0.0492 (18)	0.0518 (18)	0.0018 (14)	−0.0193 (16)	−0.0008 (14)
C10B	0.0510 (18)	0.0490 (17)	0.0394 (16)	−0.0004 (14)	−0.0090 (14)	−0.0062 (13)
C11B	0.069 (2)	0.058 (2)	0.0498 (19)	0.0130 (17)	−0.0233 (17)	−0.0114 (15)
C12B	0.101 (3)	0.070 (2)	0.094 (3)	0.027 (2)	−0.056 (2)	−0.018 (2)
C13B	0.0490 (18)	0.0441 (16)	0.0457 (17)	−0.0028 (13)	−0.0143 (15)	−0.0007 (13)
C14B	0.0511 (19)	0.0492 (17)	0.0535 (19)	−0.0024 (14)	−0.0122 (16)	−0.0058 (14)
C15B	0.0499 (19)	0.0531 (18)	0.0503 (18)	−0.0103 (15)	−0.0113 (16)	−0.0072 (14)
C16B	0.067 (2)	0.061 (2)	0.066 (2)	−0.0021 (17)	−0.0137 (19)	−0.0208 (17)
C17B	0.077 (3)	0.079 (2)	0.074 (3)	−0.006 (2)	−0.012 (2)	−0.0313 (19)
C18B	0.084 (3)	0.089 (3)	0.071 (2)	−0.015 (2)	−0.024 (2)	−0.032 (2)
C19B	0.064 (2)	0.082 (2)	0.067 (2)	−0.0052 (18)	−0.0238 (19)	−0.0199 (19)
C20B	0.053 (2)	0.0516 (17)	0.0480 (18)	−0.0096 (15)	−0.0121 (16)	−0.0074 (14)
C21B	0.0525 (19)	0.0441 (16)	0.0416 (17)	−0.0030 (14)	−0.0139 (15)	0.0002 (13)
C22B	0.058 (2)	0.070 (2)	0.056 (2)	0.0096 (17)	−0.0245 (17)	−0.0090 (16)
C23B	0.081 (2)	0.065 (2)	0.054 (2)	0.0225 (18)	−0.0256 (19)	−0.0060 (16)
C24B	0.078 (2)	0.082 (2)	0.051 (2)	0.027 (2)	−0.0206 (19)	−0.0126 (17)
C25B	0.068 (2)	0.063 (2)	0.0486 (19)	0.0104 (17)	−0.0133 (17)	0.0002 (16)
O2B	0.099 (2)	0.0923 (18)	0.0857 (19)	0.0430 (16)	−0.0306 (16)	−0.0226 (14)
O3B	0.108 (2)	0.112 (2)	0.0537 (15)	0.0459 (17)	−0.0173 (15)	−0.0233 (14)
C26B	0.070 (2)	0.062 (2)	0.060 (2)	0.0113 (18)	−0.013 (2)	−0.0101 (17)
C27B	0.107 (4)	0.125 (4)	0.063 (3)	0.032 (3)	−0.012 (3)	−0.037 (2)
C28B	0.119 (5)	0.277 (8)	0.124 (5)	−0.027 (5)	0.031 (4)	−0.060 (5)
C29B	0.210 (7)	0.267 (7)	0.069 (3)	0.102 (6)	−0.041 (4)	−0.060 (4)
C30B	0.289 (9)	0.119 (4)	0.166 (6)	0.028 (5)	−0.067 (6)	−0.073 (4)

Geometric parameters (Å, º)

O1A—C2A	1.367 (3)	O2C—C26C	1.218 (10)
O1A—C1A	1.423 (4)	O3C—C26C	1.325 (9)
N1A—C11A	1.337 (3)	O3C—C27C	1.480 (10)
N1A—C8A	1.342 (3)	C27C—C29C	1.505 (10)
N2A—C11A	1.328 (4)	C27C—C30C	1.511 (12)
N2A—C10A	1.341 (3)	C27C—C28C	1.518 (12)
N3A—C21A	1.325 (3)	C28C—H28A	0.9600
N3A—C20A	1.368 (4)	C28C—H28B	0.9600
C1A—H1AA	0.9600	C28C—H28C	0.9600
C1A—H1AB	0.9600	C29C—H29A	0.9600
C1A—H1AC	0.9600	C29C—H29B	0.9600
C2A—C7A	1.365 (4)	C29C—H29C	0.9600
C2A—C3A	1.378 (4)	C30C—H30A	0.9600
C3A—C4A	1.369 (4)	C30C—H30B	0.9600

C3A—H3AA	0.9300	C30C—H30C	0.9600
C4A—C5A	1.391 (4)	O1B—C2B	1.371 (4)
C4A—H4AA	0.9300	O1B—C1B	1.419 (4)
C5A—C6A	1.383 (4)	N1B—C11B	1.338 (4)
C5A—C8A	1.476 (3)	N1B—C8B	1.346 (3)
C6A—C7A	1.380 (4)	N2B—C11B	1.335 (4)
C6A—H6AA	0.9300	N2B—C10B	1.337 (3)
C7A—H7AA	0.9300	N3B—C21B	1.314 (3)
C8A—C9A	1.386 (4)	N3B—C20B	1.379 (3)
C9A—C10A	1.382 (3)	N4B—C21B	1.405 (3)
C9A—H9AA	0.9300	N4B—C22B	1.457 (3)
C10A—C13A	1.491 (4)	N4B—C25B	1.463 (3)
C11A—C12A	1.500 (4)	N5B—C26B	1.347 (4)
C12A—H12D	0.9600	N5B—C23B	1.454 (4)
C12A—H12E	0.9600	N5B—C24B	1.458 (4)
C12A—H12F	0.9600	C1B—H1BA	0.9600
C12A—H12X	0.9600	C1B—H1BB	0.9600
C12A—H12Y	0.9600	C1B—H1BC	0.9600
C12A—H12Z	0.9600	C2B—C3B	1.365 (4)
C13A—C14A	1.368 (4)	C2B—C7B	1.375 (4)
C13A—C21A	1.434 (4)	C3B—C4B	1.394 (4)
C14A—C15A	1.411 (4)	C3B—H3BA	0.9300
C14A—H14B	0.9300	C4B—C5B	1.379 (4)
C15A—C16A	1.404 (4)	C4B—H4BA	0.9300
C15A—C20A	1.406 (4)	C5B—C6B	1.384 (4)
C16A—C17A	1.360 (4)	C5B—C8B	1.481 (4)
C16A—H16B	0.9300	C6B—C7B	1.378 (4)
C17A—C18A	1.390 (5)	C6B—H6BA	0.9300
C17A—H17B	0.9300	C7B—H7BA	0.9300
C18A—C19A	1.353 (5)	C8B—C9B	1.379 (4)
C18A—H18B	0.9300	C9B—C10B	1.388 (4)
C19A—C20A	1.412 (4)	C9B—H9BA	0.9300
C19A—H19B	0.9300	C10B—C13B	1.486 (4)
C21A—N4A	1.397 (4)	C11B—C12B	1.503 (4)
C21A—N4C	1.422 (9)	C12B—H12A	0.9600
N4A—C22A	1.461 (5)	C12B—H12B	0.9600
N4A—C25A	1.464 (5)	C12B—H12C	0.9600
N5A—C26A	1.358 (5)	C12B—H12H	0.9600
N5A—C24A	1.452 (6)	C12B—H12I	0.9600
N5A—C23A	1.461 (6)	C12B—H12J	0.9600
C22A—C23A	1.505 (4)	C13B—C14B	1.360 (4)
C22A—H22A	0.9700	C13B—C21B	1.437 (4)
C22A—H22B	0.9700	C14B—C15B	1.413 (4)
C23A—H23A	0.9700	C14B—H14A	0.9300
C23A—H23B	0.9700	C15B—C20B	1.395 (4)
C24A—C25A	1.504 (5)	C15B—C16B	1.403 (4)
C24A—H24A	0.9700	C16B—C17B	1.362 (4)
C24A—H24B	0.9700	C16B—H16A	0.9300

C25A—H25A	0.9700	C17B—C18B	1.387 (5)
C25A—H25B	0.9700	C17B—H17A	0.9300
O2A—C26A	1.211 (5)	C18B—C19B	1.368 (4)
O3A—C26A	1.332 (5)	C18B—H18A	0.9300
O3A—C27A	1.474 (5)	C19B—C20B	1.406 (4)
C27A—C29A	1.509 (6)	C19B—H19A	0.9300
C27A—C30A	1.515 (9)	C22B—C23B	1.516 (4)
C27A—C28A	1.516 (9)	C22B—H22C	0.9700
C28A—H28D	0.9600	C22B—H22D	0.9700
C28A—H28E	0.9600	C23B—H23C	0.9700
C28A—H28F	0.9600	C23B—H23D	0.9700
C29A—H29D	0.9600	C24B—C25B	1.496 (4)
C29A—H29E	0.9600	C24B—H24C	0.9700
C29A—H29F	0.9600	C24B—H24D	0.9700
C30A—H30D	0.9600	C25B—H25C	0.9700
C30A—H30E	0.9600	C25B—H25D	0.9700
C30A—H30F	0.9600	O2B—C26B	1.211 (3)
N4C—C25C	1.464 (10)	O3B—C26B	1.327 (4)
N4C—C22C	1.468 (10)	O3B—C27B	1.466 (4)
N5C—C26C	1.364 (9)	C27B—C30B	1.460 (6)
N5C—C24C	1.442 (10)	C27B—C28B	1.495 (7)
N5C—C23C	1.474 (10)	C27B—C29B	1.502 (6)
C22C—C23C	1.508 (9)	C28B—H28G	0.9600
C22C—H22E	0.9700	C28B—H28H	0.9600
C22C—H22F	0.9700	C28B—H28I	0.9600
C23C—H23E	0.9700	C29B—H29G	0.9600
C23C—H23F	0.9700	C29B—H29H	0.9600
C24C—C25C	1.504 (10)	C29B—H29I	0.9600
C24C—H24E	0.9700	C30B—H30G	0.9600
C24C—H24F	0.9700	C30B—H30H	0.9600
C25C—H25E	0.9700	C30B—H30I	0.9600
C25C—H25F	0.9700		

C2A—O1A—C1A	117.2 (3)	C24C—C25C—H25F	109.0
C11A—N1A—C8A	116.4 (3)	H25E—C25C—H25F	107.8
C11A—N2A—C10A	116.2 (2)	C26C—O3C—C27C	119.5 (11)
C21A—N3A—C20A	118.1 (3)	O2C—C26C—O3C	126.0 (12)
O1A—C1A—H1AA	109.5	O2C—C26C—N5C	119.8 (11)
O1A—C1A—H1AB	109.5	O3C—C26C—N5C	113.9 (10)
H1AA—C1A—H1AB	109.5	O3C—C27C—C29C	100.6 (10)
O1A—C1A—H1AC	109.5	O3C—C27C—C30C	110.0 (12)
H1AA—C1A—H1AC	109.5	C29C—C27C—C30C	113.1 (15)
H1AB—C1A—H1AC	109.5	O3C—C27C—C28C	109.0 (11)
C7A—C2A—O1A	124.7 (3)	C29C—C27C—C28C	110.5 (14)
C7A—C2A—C3A	119.6 (3)	C30C—C27C—C28C	112.9 (14)
O1A—C2A—C3A	115.7 (3)	C27C—C28C—H28A	109.5
C4A—C3A—C2A	120.5 (3)	C27C—C28C—H28B	109.5
C4A—C3A—H3AA	119.7	H28A—C28C—H28B	109.5

C2A—C3A—H3AA	119.7	C27C—C28C—H28C	109.5
C3A—C4A—C5A	121.2 (3)	H28A—C28C—H28C	109.5
C3A—C4A—H4AA	119.4	H28B—C28C—H28C	109.5
C5A—C4A—H4AA	119.4	C27C—C29C—H29A	109.5
C6A—C5A—C4A	117.0 (3)	C27C—C29C—H29B	109.5
C6A—C5A—C8A	122.4 (3)	H29A—C29C—H29B	109.5
C4A—C5A—C8A	120.7 (3)	C27C—C29C—H29C	109.5
C7A—C6A—C5A	122.1 (3)	H29A—C29C—H29C	109.5
C7A—C6A—H6AA	119.0	H29B—C29C—H29C	109.5
C5A—C6A—H6AA	119.0	C27C—C30C—H30A	109.5
C2A—C7A—C6A	119.6 (3)	C27C—C30C—H30B	109.5
C2A—C7A—H7AA	120.2	H30A—C30C—H30B	109.5
C6A—C7A—H7AA	120.2	C27C—C30C—H30C	109.5
N1A—C8A—C9A	120.5 (2)	H30A—C30C—H30C	109.5
N1A—C8A—C5A	116.4 (2)	H30B—C30C—H30C	109.5
C9A—C8A—C5A	123.1 (3)	C2B—O1B—C1B	117.6 (3)
C10A—C9A—C8A	118.7 (3)	C11B—N1B—C8B	116.8 (3)
C10A—C9A—H9AA	120.7	C11B—N2B—C10B	116.5 (2)
C8A—C9A—H9AA	120.7	C21B—N3B—C20B	118.3 (3)
N2A—C10A—C9A	121.1 (3)	C21B—N4B—C22B	117.4 (2)
N2A—C10A—C13A	115.1 (2)	C21B—N4B—C25B	116.1 (2)
C9A—C10A—C13A	123.4 (3)	C22B—N4B—C25B	110.0 (2)
N2A—C11A—N1A	127.1 (3)	C26B—N5B—C23B	118.7 (2)
N2A—C11A—C12A	116.7 (3)	C26B—N5B—C24B	121.9 (3)
N1A—C11A—C12A	116.2 (3)	C23B—N5B—C24B	114.9 (2)
C11A—C12A—H12D	109.5	O1B—C1B—H1BA	109.5
C11A—C12A—H12E	109.5	O1B—C1B—H1BB	109.5
H12D—C12A—H12E	109.5	H1BA—C1B—H1BB	109.5
C11A—C12A—H12F	109.5	O1B—C1B—H1BC	109.5
H12D—C12A—H12F	109.5	H1BA—C1B—H1BC	109.5
H12E—C12A—H12F	109.5	H1BB—C1B—H1BC	109.5
C11A—C12A—H12X	109.5	C3B—C2B—O1B	124.4 (3)
H12D—C12A—H12X	141.1	C3B—C2B—C7B	120.3 (3)
H12E—C12A—H12X	56.3	O1B—C2B—C7B	115.3 (3)
H12F—C12A—H12X	56.3	C2B—C3B—C4B	119.3 (3)
C11A—C12A—H12Y	109.5	C2B—C3B—H3BA	120.3
H12D—C12A—H12Y	56.3	C4B—C3B—H3BA	120.3
H12E—C12A—H12Y	141.1	C5B—C4B—C3B	121.5 (3)
H12F—C12A—H12Y	56.3	C5B—C4B—H4BA	119.2
H12X—C12A—H12Y	109.5	C3B—C4B—H4BA	119.2
C11A—C12A—H12Z	109.5	C4B—C5B—C6B	117.4 (3)
H12D—C12A—H12Z	56.3	C4B—C5B—C8B	121.4 (3)
H12E—C12A—H12Z	56.3	C6B—C5B—C8B	121.2 (3)
H12F—C12A—H12Z	141.1	C7B—C6B—C5B	121.6 (3)
H12X—C12A—H12Z	109.5	C7B—C6B—H6BA	119.2
H12Y—C12A—H12Z	109.5	C5B—C6B—H6BA	119.2
C14A—C13A—C21A	116.9 (3)	C2B—C7B—C6B	119.7 (3)
C14A—C13A—C10A	117.3 (3)	C2B—C7B—H7BA	120.1

C21A—C13A—C10A	125.5 (2)	C6B—C7B—H7BA	120.1
C13A—C14A—C15A	121.8 (3)	N1B—C8B—C9B	120.4 (3)
C13A—C14A—H14B	119.1	N1B—C8B—C5B	116.2 (3)
C15A—C14A—H14B	119.1	C9B—C8B—C5B	123.3 (2)
C16A—C15A—C20A	119.9 (3)	C8B—C9B—C10B	118.7 (3)
C16A—C15A—C14A	123.9 (3)	C8B—C9B—H9BA	120.6
C20A—C15A—C14A	116.2 (3)	C10B—C9B—H9BA	120.6
C17A—C16A—C15A	121.2 (4)	N2B—C10B—C9B	121.1 (3)
C17A—C16A—H16B	119.4	N2B—C10B—C13B	116.5 (2)
C15A—C16A—H16B	119.4	C9B—C10B—C13B	122.2 (3)
C16A—C17A—C18A	118.6 (3)	N2B—C11B—N1B	126.4 (3)
C16A—C17A—H17B	120.7	N2B—C11B—C12B	116.8 (3)
C18A—C17A—H17B	120.7	N1B—C11B—C12B	116.8 (3)
C19A—C18A—C17A	122.1 (4)	C11B—C12B—H12A	109.5
C19A—C18A—H18B	118.9	C11B—C12B—H12B	109.5
C17A—C18A—H18B	118.9	H12A—C12B—H12B	109.5
C18A—C19A—C20A	120.5 (4)	C11B—C12B—H12C	109.5
C18A—C19A—H19B	119.7	H12A—C12B—H12C	109.5
C20A—C19A—H19B	119.7	H12B—C12B—H12C	109.5
N3A—C20A—C15A	123.1 (3)	C11B—C12B—H12H	109.5
N3A—C20A—C19A	119.2 (3)	H12A—C12B—H12H	141.1
C15A—C20A—C19A	117.6 (3)	H12B—C12B—H12H	56.3
N3A—C21A—N4A	115.7 (4)	H12C—C12B—H12H	56.3
N3A—C21A—N4C	122.0 (13)	C11B—C12B—H12I	109.5
N3A—C21A—C13A	123.2 (3)	H12A—C12B—H12I	56.3
N4A—C21A—C13A	121.0 (4)	H12B—C12B—H12I	141.1
N4C—C21A—C13A	114.5 (12)	H12C—C12B—H12I	56.3
C21A—N4A—C22A	114.4 (5)	H12H—C12B—H12I	109.5
C21A—N4A—C25A	116.2 (5)	C11B—C12B—H12J	109.5
C22A—N4A—C25A	109.8 (4)	H12A—C12B—H12J	56.3
C26A—N5A—C24A	118.7 (4)	H12B—C12B—H12J	56.3
C26A—N5A—C23A	124.3 (4)	H12C—C12B—H12J	141.1
C24A—N5A—C23A	114.2 (3)	H12H—C12B—H12J	109.5
N4A—C22A—C23A	111.3 (4)	H12I—C12B—H12J	109.5
N4A—C22A—H22A	109.4	C14B—C13B—C21B	116.9 (3)
C23A—C22A—H22A	109.4	C14B—C13B—C10B	118.3 (3)
N4A—C22A—H22B	109.4	C21B—C13B—C10B	124.6 (3)
C23A—C22A—H22B	109.4	C13B—C14B—C15B	121.7 (3)
H22A—C22A—H22B	108.0	C13B—C14B—H14A	119.1
N5A—C23A—C22A	109.9 (4)	C15B—C14B—H14A	119.1
N5A—C23A—H23A	109.7	C20B—C15B—C16B	120.3 (3)
C22A—C23A—H23A	109.7	C20B—C15B—C14B	116.7 (3)
N5A—C23A—H23B	109.7	C16B—C15B—C14B	123.0 (3)
C22A—C23A—H23B	109.7	C17B—C16B—C15B	119.8 (3)
H23A—C23A—H23B	108.2	C17B—C16B—H16A	120.1
N5A—C24A—C25A	110.7 (4)	C15B—C16B—H16A	120.1
N5A—C24A—H24A	109.5	C16B—C17B—C18B	120.3 (3)
C25A—C24A—H24A	109.5	C16B—C17B—H17A	119.9

N5A—C24A—H24B	109.5	C18B—C17B—H17A	119.9
C25A—C24A—H24B	109.5	C19B—C18B—C17B	121.0 (4)
H24A—C24A—H24B	108.1	C19B—C18B—H18A	119.5
N4A—C25A—C24A	109.0 (4)	C17B—C18B—H18A	119.5
N4A—C25A—H25A	109.9	C18B—C19B—C20B	120.0 (3)
C24A—C25A—H25A	109.9	C18B—C19B—H19A	120.0
N4A—C25A—H25B	109.9	C20B—C19B—H19A	120.0
C24A—C25A—H25B	109.9	N3B—C20B—C15B	122.7 (3)
H25A—C25A—H25B	108.3	N3B—C20B—C19B	118.6 (3)
C26A—O3A—C27A	120.1 (4)	C15B—C20B—C19B	118.7 (3)
O2A—C26A—O3A	125.9 (4)	N3B—C21B—N4B	117.5 (3)
O2A—C26A—N5A	123.2 (4)	N3B—C21B—C13B	123.2 (3)
O3A—C26A—N5A	110.9 (4)	N4B—C21B—C13B	119.2 (3)
O3A—C27A—C29A	101.2 (4)	N4B—C22B—C23B	109.1 (3)
O3A—C27A—C30A	109.8 (4)	N4B—C22B—H22C	109.9
C29A—C27A—C30A	111.7 (6)	C23B—C22B—H22C	109.9
O3A—C27A—C28A	110.4 (5)	N4B—C22B—H22D	109.9
C29A—C27A—C28A	110.7 (6)	C23B—C22B—H22D	109.9
C30A—C27A—C28A	112.5 (6)	H22C—C22B—H22D	108.3
C27A—C28A—H28D	109.5	N5B—C23B—C22B	110.7 (2)
C27A—C28A—H28E	109.5	N5B—C23B—H23C	109.5
H28D—C28A—H28E	109.5	C22B—C23B—H23C	109.5
C27A—C28A—H28F	109.5	N5B—C23B—H23D	109.5
H28D—C28A—H28F	109.5	C22B—C23B—H23D	109.5
H28E—C28A—H28F	109.5	H23C—C23B—H23D	108.1
C27A—C29A—H29D	109.5	N5B—C24B—C25B	110.4 (3)
C27A—C29A—H29E	109.5	N5B—C24B—H24C	109.6
H29D—C29A—H29E	109.5	C25B—C24B—H24C	109.6
C27A—C29A—H29F	109.5	N5B—C24B—H24D	109.6
H29D—C29A—H29F	109.5	C25B—C24B—H24D	109.6
H29E—C29A—H29F	109.5	H24C—C24B—H24D	108.1
C27A—C30A—H30D	109.5	N4B—C25B—C24B	110.4 (2)
C27A—C30A—H30E	109.5	N4B—C25B—H25C	109.6
H30D—C30A—H30E	109.5	C24B—C25B—H25C	109.6
C27A—C30A—H30F	109.5	N4B—C25B—H25D	109.6
H30D—C30A—H30F	109.5	C24B—C25B—H25D	109.6
H30E—C30A—H30F	109.5	H25C—C25B—H25D	108.1
C21A—N4C—C25C	119.0 (17)	C26B—O3B—C27B	122.9 (3)
C21A—N4C—C22C	119.2 (17)	O2B—C26B—O3B	124.8 (3)
C25C—N4C—C22C	108.6 (12)	O2B—C26B—N5B	123.2 (3)
C26C—N5C—C24C	123.0 (11)	O3B—C26B—N5B	112.0 (3)
C26C—N5C—C23C	120.0 (11)	C30B—C27B—O3B	112.3 (4)
C24C—N5C—C23C	111.6 (11)	C30B—C27B—C28B	110.3 (5)
N4C—C22C—C23C	112.8 (12)	O3B—C27B—C28B	107.3 (4)
N4C—C22C—H22E	109.0	C30B—C27B—C29B	112.9 (5)
C23C—C22C—H22E	109.0	O3B—C27B—C29B	102.1 (3)
N4C—C22C—H22F	109.0	C28B—C27B—C29B	111.7 (5)
C23C—C22C—H22F	109.0	C27B—C28B—H28G	109.5

H22E—C22C—H22F	107.8	C27B—C28B—H28H	109.5
N5C—C23C—C22C	109.2 (12)	H28G—C28B—H28H	109.5
N5C—C23C—H23E	109.8	C27B—C28B—H28I	109.5
C22C—C23C—H23E	109.8	H28G—C28B—H28I	109.5
N5C—C23C—H23F	109.8	H28H—C28B—H28I	109.5
C22C—C23C—H23F	109.8	C27B—C29B—H29G	109.5
H23E—C23C—H23F	108.3	C27B—C29B—H29H	109.5
N5C—C24C—C25C	111.2 (12)	H29G—C29B—H29H	109.5
N5C—C24C—H24E	109.4	C27B—C29B—H29I	109.5
C25C—C24C—H24E	109.4	H29G—C29B—H29I	109.5
N5C—C24C—H24F	109.4	H29H—C29B—H29I	109.5
C25C—C24C—H24F	109.4	C27B—C30B—H30G	109.5
H24E—C24C—H24F	108.0	C27B—C30B—H30H	109.5
N4C—C25C—C24C	113.0 (12)	H30G—C30B—H30H	109.5
N4C—C25C—H25E	109.0	C27B—C30B—H30I	109.5
C24C—C25C—H25E	109.0	H30G—C30B—H30I	109.5
N4C—C25C—H25F	109.0	H30H—C30B—H30I	109.5

C1A—O1A—C2A—C7A	−3.2 (5)	C23C—N5C—C24C—C25C	55 (2)
C1A—O1A—C2A—C3A	176.0 (3)	C21A—N4C—C25C—C24C	−165 (3)
C7A—C2A—C3A—C4A	0.1 (5)	C22C—N4C—C25C—C24C	54 (2)
O1A—C2A—C3A—C4A	−179.2 (3)	N5C—C24C—C25C—N4C	−55 (2)
C2A—C3A—C4A—C5A	0.1 (5)	C27C—O3C—C26C—O2C	−2 (3)
C3A—C4A—C5A—C6A	0.0 (4)	C27C—O3C—C26C—N5C	171.3 (17)
C3A—C4A—C5A—C8A	179.8 (3)	C24C—N5C—C26C—O2C	−170 (2)
C4A—C5A—C6A—C7A	−0.4 (4)	C23C—N5C—C26C—O2C	−18 (3)
C8A—C5A—C6A—C7A	179.8 (3)	C24C—N5C—C26C—O3C	16 (3)
O1A—C2A—C7A—C6A	178.8 (3)	C23C—N5C—C26C—O3C	168.1 (19)
C3A—C2A—C7A—C6A	−0.4 (5)	C26C—O3C—C27C—C29C	−176.8 (17)
C5A—C6A—C7A—C2A	0.5 (5)	C26C—O3C—C27C—C30C	64 (2)
C11A—N1A—C8A—C9A	−1.7 (4)	C26C—O3C—C27C—C28C	−61 (2)
C11A—N1A—C8A—C5A	179.9 (2)	C1B—O1B—C2B—C3B	−2.6 (5)
C6A—C5A—C8A—N1A	−160.9 (3)	C1B—O1B—C2B—C7B	178.5 (3)
C4A—C5A—C8A—N1A	19.3 (4)	O1B—C2B—C3B—C4B	178.6 (3)
C6A—C5A—C8A—C9A	20.8 (4)	C7B—C2B—C3B—C4B	−2.7 (5)
C4A—C5A—C8A—C9A	−159.0 (3)	C2B—C3B—C4B—C5B	−1.0 (5)
N1A—C8A—C9A—C10A	1.1 (4)	C3B—C4B—C5B—C6B	3.7 (5)
C5A—C8A—C9A—C10A	179.4 (2)	C3B—C4B—C5B—C8B	−174.0 (3)
C11A—N2A—C10A—C9A	−0.6 (4)	C4B—C5B—C6B—C7B	−2.9 (4)
C11A—N2A—C10A—C13A	172.7 (2)	C8B—C5B—C6B—C7B	174.9 (3)
C8A—C9A—C10A—N2A	0.1 (4)	C3B—C2B—C7B—C6B	3.5 (5)
C8A—C9A—C10A—C13A	−172.7 (2)	O1B—C2B—C7B—C6B	−177.6 (3)
C10A—N2A—C11A—N1A	0.0 (5)	C5B—C6B—C7B—C2B	−0.7 (5)
C10A—N2A—C11A—C12A	−178.7 (3)	C11B—N1B—C8B—C9B	−1.0 (4)
C8A—N1A—C11A—N2A	1.2 (5)	C11B—N1B—C8B—C5B	−178.9 (3)
C8A—N1A—C11A—C12A	179.9 (3)	C4B—C5B—C8B—N1B	−174.6 (3)
N2A—C10A—C13A—C14A	−29.4 (4)	C6B—C5B—C8B—N1B	7.8 (4)
C9A—C10A—C13A—C14A	143.8 (3)	C4B—C5B—C8B—C9B	7.6 (4)

N2A—C10A—C13A—C21A	157.0 (3)	C6B—C5B—C8B—C9B	−170.1 (3)
C9A—C10A—C13A—C21A	−29.9 (4)	N1B—C8B—C9B—C10B	1.9 (4)
C21A—C13A—C14A—C15A	2.8 (4)	C5B—C8B—C9B—C10B	179.7 (3)
C10A—C13A—C14A—C15A	−171.5 (2)	C11B—N2B—C10B—C9B	0.3 (4)
C13A—C14A—C15A—C16A	−176.7 (3)	C11B—N2B—C10B—C13B	174.7 (3)
C13A—C14A—C15A—C20A	4.0 (4)	C8B—C9B—C10B—N2B	−1.6 (4)
C20A—C15A—C16A—C17A	0.1 (4)	C8B—C9B—C10B—C13B	−175.6 (2)
C14A—C15A—C16A—C17A	−179.2 (3)	C10B—N2B—C11B—N1B	0.7 (5)
C15A—C16A—C17A—C18A	2.2 (5)	C10B—N2B—C11B—C12B	−179.2 (3)
C16A—C17A—C18A—C19A	−2.0 (5)	C8B—N1B—C11B—N2B	−0.4 (5)
C17A—C18A—C19A—C20A	−0.5 (5)	C8B—N1B—C11B—C12B	179.6 (3)
C21A—N3A—C20A—C15A	3.1 (4)	N2B—C10B—C13B—C14B	−37.4 (4)
C21A—N3A—C20A—C19A	179.1 (3)	C9B—C10B—C13B—C14B	136.9 (3)
C16A—C15A—C20A—N3A	173.4 (3)	N2B—C10B—C13B—C21B	148.4 (3)
C14A—C15A—C20A—N3A	−7.2 (4)	C9B—C10B—C13B—C21B	−37.4 (4)
C16A—C15A—C20A—C19A	−2.6 (4)	C21B—C13B—C14B—C15B	3.9 (4)
C14A—C15A—C20A—C19A	176.8 (3)	C10B—C13B—C14B—C15B	−170.8 (2)
C18A—C19A—C20A—N3A	−173.4 (3)	C13B—C14B—C15B—C20B	2.4 (4)
C18A—C19A—C20A—C15A	2.8 (4)	C13B—C14B—C15B—C16B	−179.5 (3)
C20A—N3A—C21A—N4A	−176.8 (4)	C20B—C15B—C16B—C17B	−0.3 (5)
C20A—N3A—C21A—N4C	−168.5 (17)	C14B—C15B—C16B—C17B	−178.2 (3)
C20A—N3A—C21A—C13A	4.4 (4)	C15B—C16B—C17B—C18B	1.7 (5)
C14A—C13A—C21A—N3A	−7.3 (4)	C16B—C17B—C18B—C19B	−1.4 (5)
C10A—C13A—C21A—N3A	166.4 (2)	C17B—C18B—C19B—C20B	−0.2 (5)
C14A—C13A—C21A—N4A	173.9 (4)	C21B—N3B—C20B—C15B	3.7 (4)
C10A—C13A—C21A—N4A	−12.4 (6)	C21B—N3B—C20B—C19B	−179.6 (3)
C14A—C13A—C21A—N4C	166.0 (16)	C16B—C15B—C20B—N3B	175.4 (3)
C10A—C13A—C21A—N4C	−20.3 (17)	C14B—C15B—C20B—N3B	−6.5 (4)
N3A—C21A—N4A—C22A	119.7 (5)	C16B—C15B—C20B—C19B	−1.3 (4)
C13A—C21A—N4A—C22A	−61.4 (6)	C14B—C15B—C20B—C19B	176.8 (3)
N3A—C21A—N4A—C25A	−9.8 (7)	C18B—C19B—C20B—N3B	−175.3 (3)
C13A—C21A—N4A—C25A	169.0 (4)	C18B—C19B—C20B—C15B	1.6 (5)
C21A—N4A—C22A—C23A	167.0 (6)	C20B—N3B—C21B—N4B	−177.9 (2)
C25A—N4A—C22A—C23A	−60.2 (6)	C20B—N3B—C21B—C13B	3.3 (4)
C26A—N5A—C23A—C22A	147.7 (5)	C22B—N4B—C21B—N3B	−9.6 (4)
C24A—N5A—C23A—C22A	−51.5 (5)	C25B—N4B—C21B—N3B	123.5 (3)
N4A—C22A—C23A—N5A	54.0 (6)	C22B—N4B—C21B—C13B	169.3 (2)
C26A—N5A—C24A—C25A	−144.1 (4)	C25B—N4B—C21B—C13B	−57.7 (3)
C23A—N5A—C24A—C25A	54.0 (5)	C14B—C13B—C21B—N3B	−7.0 (4)
C21A—N4A—C25A—C24A	−167.2 (6)	C10B—C13B—C21B—N3B	167.3 (2)
C22A—N4A—C25A—C24A	61.0 (5)	C14B—C13B—C21B—N4B	174.1 (2)
N5A—C24A—C25A—N4A	−57.5 (5)	C10B—C13B—C21B—N4B	−11.5 (4)
C27A—O3A—C26A—O2A	4.9 (6)	C21B—N4B—C22B—C23B	−162.8 (2)
C27A—O3A—C26A—N5A	−175.2 (4)	C25B—N4B—C22B—C23B	61.5 (3)
C24A—N5A—C26A—O2A	8.5 (6)	C26B—N5B—C23B—C22B	−152.0 (3)
C23A—N5A—C26A—O2A	168.5 (4)	C24B—N5B—C23B—C22B	51.4 (4)
C24A—N5A—C26A—O3A	−171.4 (3)	N4B—C22B—C23B—N5B	−55.4 (4)
C23A—N5A—C26A—O3A	−11.4 (6)	C26B—N5B—C24B—C25B	153.4 (3)

C26A—O3A—C27A—C29A	176.5 (4)	C23B—N5B—C24B—C25B	−50.8 (4)
C26A—O3A—C27A—C30A	−65.3 (6)	C21B—N4B—C25B—C24B	161.7 (3)
C26A—O3A—C27A—C28A	59.2 (7)	C22B—N4B—C25B—C24B	−61.9 (3)
N3A—C21A—N4C—C25C	−15 (3)	N5B—C24B—C25B—N4B	54.8 (4)
C13A—C21A—N4C—C25C	171.5 (19)	C27B—O3B—C26B—O2B	3.2 (6)
N3A—C21A—N4C—C22C	121 (2)	C27B—O3B—C26B—N5B	−176.7 (3)
C13A—C21A—N4C—C22C	−52 (3)	C23B—N5B—C26B—O2B	13.4 (5)
C21A—N4C—C22C—C23C	163 (3)	C24B—N5B—C26B—O2B	168.3 (3)
C25C—N4C—C22C—C23C	−56 (2)	C23B—N5B—C26B—O3B	−166.7 (3)
C26C—N5C—C23C—C22C	149 (2)	C24B—N5B—C26B—O3B	−11.8 (5)
C24C—N5C—C23C—C22C	−56 (2)	C26B—O3B—C27B—C30B	−57.1 (6)
N4C—C22C—C23C—N5C	58 (2)	C26B—O3B—C27B—C28B	64.2 (5)
C26C—N5C—C24C—C25C	−151 (2)	C26B—O3B—C27B—C29B	−178.2 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7*B*—H7*BA*···O2*B*^{i}	0.93	2.40	3.141 (2)	136

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