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1,4-Dibenzyl-6-chloroquinoxaline-2,3(1*H*,4*H*)dione

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The title compound, $C_{22}H_{17}CIN_2O_2$, crystallizes with two independent molecules (*A* and *B*) in the asymmetric unit. The 6-chloroquinoxaline-2,3(1*H*,4*H*)-dione ring system is essentially planar. The dihedral angles between the mean planes of the 6-chloroquinoxaline-2,3(1*H*,4*H*)-dione ring and the phenyl rings of the benzyl substituents in the two molecules are 68.34 and 73.8 (7)° for *A*, and 73.8 (5) and 80.7 (1)° for *B*, so that these rings point away from the quinoxaline ring system. In the crystal, weak $C-H\cdots$ O hydrogen bonds and $\pi-\pi$ stacking interactions link the molecules into a three-dimensional network.



Structure description

Quinoxaline derivatives find use as anticancer (Noolvi *et al.*, 2011), antidiabetic (Bahekar *et al.*, 2007), antifungal (Xu and Fan, 2011), antiviral (Caia *et al.*, 2008) and anti-inflammatory agents (Yan *et al.*, 2007). As part of our work in this area, the synthesis and structure of the title compound, 1,4-dibenzyl-6-chloroquinoxaline-2,3(1H,4H)-dione are reported here.

The title compound crystallizes with two independent molecules (A and B) in the asymmetric unit (Fig. 1). The 6-chloroquinoxaline-2,3(1H,4H)-dione unit is essentially planar. The maximum r.m.s. deviation from the mean plane through the non-H atoms of ring A (N1A/C1A/C2A/N2A/C3A/C8A/C7A/C5A/C4A) is 0.053 (2) Å for N2A and for ring B (N1B/C1B/C2B/N2B/C3B/C8B/C7B/C5B/C4B) is 0.096 (2) Å for N2B. The dihedral angles between the mean plane of the 6-chloroquinoxaline-2,3(1H,4H)-dione ring and its pendant phenyl rings are 68.3 (4) and 73.8 (7)° in molecule A, and 73.8 (5) and 80.7 (1)° in molecule B. The phenyl rings of the benzyl substituents in both molecules





Figure 1

The molecular structure of the title compound, showing the atomnumbering scheme for molecules A and B, and 30% probability displacement ellipsoids for the non-H atoms. Dashed lines indicate weak $C7B-H7B\cdots O2A$ and $C18B-H18B\cdots O1A$ intermolecular interactions within the asymmetric unit.

are inclined similarly, pointing away from the 6-chloroquinoxaline-2,3(1*H*,4*H*)-dione ring system. In the crystal, the two unique molecules are linked by weak $C7B-H7B\cdots O2A$ and $C18B-H18B\cdots O1A$ interactions (Table 1) within the asymmetric unit (Fig. 1). Additional $C-H\cdots O$ hydrogen bonds, together with $\pi-\pi$ stacking interactions [*Cg2-Cg7*ⁱⁱ = 3.6611 (14) Å; symmetry code: (ii) x, 1 + y, z; *Cg2* and *Cg7* are the centroids of the C3*A*-C8*A* and C3*B*-C8*B* rings, respectively], link the molecules into a three-dimensional network (Fig. 2).

Synthesis and crystallization

To a solution of 6-chloroquinoxaline-2,3(1H,4H)-dione (0.3 g, 1.53 mmol) was added a DMF (20 ml) solution of potassium carbonate (0.53 g, 3.84 mmol), tetra-*n*-butylammonium bromide (0.07 g, 0.23 mmol) and benzyl chloride (0.44 ml, 3.79 mmol). Stirring was continued at room temperature for 36 h. The mixture was filtered and the solvent removed under reduced pressure. The residue obtained was dissolved in dichloromethane. The remaining salts were extracted with distilled water and the resulting mixture was chromato-



Figure 2

The packing of the title compound, viewed along the *a* axis. Dashed lines indicate intermolecular $C-H\cdots O$ interactions. H atoms not involved in the packing have been omitted for clarity.

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

$D - H \cdots A$	$D-\mathrm{H}$	$H \cdot \cdot \cdot A$	$D \cdots A$	$D - H \cdots A$
$C7A - H7A \cdots O2B^{i}$	0.93	2.48	3.323 (3)	151
$C22A - H22A \cdots O1B^{i}$	0.93	2.60	3.454 (3)	154
$C7B - H7B \cdots O2A$	0.93	2.43	3.151 (3)	135
$C18B - H18B \cdots O1A$	0.93	2.72	3.353 (3)	126

Symmetry code: (i) $x, -y + \frac{1}{2}, z + \frac{1}{2}$.

Table 2	
Experimental	details.

$C_{22}H_{17}ClN_2O_2$
376.82
Monoclinic, I2/a
293
29.2234 (4), 8.3076 (2), 31.0407 (5)
101.859 (2)
7375.1 (2)
16
Cu Ka
1.99
$0.28 \times 0.24 \times 0.12$
Rigaku Oxford Diffraction
Multi-scan (<i>CrysAlis PRO</i> ; Rigaku Oxford Diffraction, 2015)
0.500, 1.000
14412, 6996, 5661
0.022
0.614
0.053, 0.156, 1.04
6996
487
H-atom parameters constrained
0.73, -0.37

Computer programs: CrysAlis PRO (Rigaku Oxford Diffraction, 2015), SHELXT (Sheldrick, 2015a), SHELXL2014 (Sheldrick, 2015b) and OLEX2 (Dolomanov et al., 2009).

graphed on a silica-gel column (eluent: ethyl acetate-hexane 1:2 v/v) to give the product in 87% yield. The compound was recrystallized from mixed solvents of dichloromethane-hexane (1:1 v/v) to give yellow crystals.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

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full crystallographic data

IUCrData (2017). **2**, x170901 [https://doi.org/10.1107/S2414314617009014]

1,4-Dibenzyl-6-chloroquinoxaline-2,3(1H,4H)-dione

Ali El Janati, Youssef Kandri Rodi, Jerry P. Jasinski, Manpreet Kaur, Younes Ouzidan and El Mokhtar Essassi

1,4-Dibenzyl-6-chloroguinoxaline-2,3(1H,4H)-dione

Crystal data

C22H17ClN2O2 $M_r = 376.82$ Monoclinic, *I2/a* a = 29.2234 (4) Å b = 8.3076 (2) Å c = 31.0407 (5) Å $\beta = 101.859 \ (2)^{\circ}$ V = 7375.1 (2) Å³ Z = 16

Data collection

Rigaku Oxford Diffraction	$T_{\rm min} = 0.500, T_{\rm max}$
diffractometer	14412 measured
Radiation source: fine-focus sealed X-ray tube,	6996 independent
Enhance (Cu) X-ray Source	5661 reflections
Graphite monochromator	$R_{\rm int} = 0.022$
Detector resolution: 16.0416 pixels mm ⁻¹	$\theta_{\rm max} = 71.3^{\circ}, \theta_{\rm min} =$
ω scans	$h = -35 \rightarrow 25$
Absorption correction: multi-scan	$k = -10 \rightarrow 9$
(CrysAlis PRO; Rigaku Oxford Diffraction,	$l = -37 \rightarrow 38$
2015)	

Refinement

Refinement on F^2 Least-squares matrix: full $R[F^2 > 2\sigma(F^2)] = 0.053$ $wR(F^2) = 0.156$ S = 1.046996 reflections 487 parameters 0 restraints Primary atom site location: dual

F(000) = 3136 $D_{\rm x} = 1.358 {\rm Mg} {\rm m}^{-3}$ Cu *K* α radiation, $\lambda = 1.54184$ Å Cell parameters from 6649 reflections $\theta = 4.6 - 71.4^{\circ}$ $\mu = 1.99 \text{ mm}^{-1}$ T = 293 KPrism, orange $0.28 \times 0.24 \times 0.12$ mm

= 1.000reflections t reflections with $I > 2\sigma(I)$ = 3.8°

Hydrogen site location: inferred from neighbouring sites H-atom parameters constrained $w = 1/[\sigma^2(F_0^2) + (0.0814P)^2 + 5.5513P]$ where $P = (F_0^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\rm max} = 0.001$ $\Delta \rho_{\rm max} = 0.73 \text{ e} \text{ Å}^{-3}$ $\Delta \rho_{\rm min} = -0.37 \ {\rm e} \ {\rm \AA}^{-3}$

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.

j j <th></th> <th>r</th> <th>V</th> <th>7</th> <th>Uine*/Ular</th>		r	V	7	Uine*/Ular
CIA 0.5326 (7) 0.125 (3) 0.4723 (6) 0.0740 (6)02A 0.45326 (7) 0.125 (3) 0.43236 (6) 0.0655 (5)NIA 0.55925 (6) 0.1082 (2) 0.54560 (6) 0.0477 (4)N2A 0.48818 (6) 0.3198 (2) 0.55775 (6) 0.0454 (4)CIA 0.59025 (6) 0.182 (2) 0.55975 (6) 0.0454 (4)CIA 0.53026 (7) 0.0224 (6) 0.0224 (6)C2A 0.49289 (8) 0.2857 (3) 0.51596 (7) 0.0933 (5)C3A 0.51820 (7) 0.2548 (2) 0.59492 (7) 0.4048 (4)C4A 0.554340 (7) 0.2548 (2) 0.59492 (7) 0.4048 (4)C5A 0.5851 (7) 0.0933 (3) 0.62590 (7) 0.4770 (5)H5A 0.6100 0.0268 0.6224 $0.057*$ C6A 0.57996 (8) 0.1356 (3) 0.6737 (7) 0.0451 (5)H7A 0.5406 (8) 0.2333 (3) 0.67406 (7) 0.0472 (5)H7A 0.5406 (8) 0.2594 0.7024 $0.057*$ C8A 0.51320 (7) 0.0451 (5)(5)H8A 0.4885 0.3565 0.6416 $0.054*$ C9A 0.59406 (9) -0.0137 (3) 0.5406 (8) 0.0578 (6)C11A 0.6778 (1) 0.0688 (10)(1)H9AB 0.5937 -0.1007 0.5612 $0.071*$ H9AB 0.5937 -0.1007 0.5612 $0.071*$ H9AA 0.4728 (9) 0.0527 (3) 0.114	<u></u>	0.62007.(2)	0.06298.(9)	0.71203 (2)	0.0677.(2)
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NAA $0.4816 (0)$ $0.5196 (2)$ $0.53775 (0)$ $0.0494 (4)$ C1A $0.53004 (8)$ $0.1662 (3)$ $0.5596 (7)$ $0.0524 (6)$ C2A $0.4289 (8)$ $0.2857 (3)$ $0.51596 (7)$ $0.0408 (4)$ C3A $0.51820 (7)$ $0.22548 (2)$ $0.59492 (7)$ $0.0408 (4)$ C5A $0.55440 (7)$ $0.1519 (3)$ $0.55911 (7)$ $0.0422 (4)$ C5A $0.58551 (7)$ $0.0938 (3)$ $0.62590 (7)$ $0.0470 (5)$ H5A 0.6100 0.0268 0.6224 0.056^* C6A $0.57996 (8)$ $0.1356 (3)$ $0.66737 (7)$ $0.0447 (5)$ T7A $0.54401 (8)$ $0.2333 (3)$ $0.67408 (7)$ $0.0472 (5)$ H7A 0.5406 0.2294 0.7024 0.057^* C8A $0.51320 (7)$ $0.2914 (3)$ $0.63765 (7)$ $0.0451 (5)$ H8A 0.4885 0.3565 0.6416 $0.054*$ C9A $0.5990 (6)$ $-0.0137 (3)$ $0.54046 (9)$ $0.0590 (6)$ H9AA 0.5873 -0.1007 0.5612 $0.071*$ H9AB 0.5937 -0.1007 $0.5468 (8)$ $0.0578 (6)$ C11A 0.6738 -0.1102 0.5917 $0.10882 (10)$ H11A 0.6738 $-0.1020 (5)$ $0.5770 (11)$ $0.0882 (10)$ H11A $0.7324 (11)$ $0.1720 (7)$ $0.55627 (13)$ $0.1144 (16)$ H12A $0.7226 (13)$ $0.5124 (9)$ $0.0678 (10)$ H12A $0.7268 (12)$ 0.3315 0.5110 $0.163*$ C15A <td>NIA N2A</td> <td>0.33923(0)</td> <td>0.1082(2)</td> <td>0.54050(0)</td> <td>0.0477(4)</td>	NIA N2A	0.33923(0)	0.1082(2)	0.54050(0)	0.0477(4)
C1A 0.30304 (s) 0.1002 (s) 0.30505 (r) 0.00503 (s)C2A 0.49228 (s) 0.2587 (3) 0.51596 (7) 0.0503 (s)C3A 0.51820 (7) 0.2548 (2) 0.59492 (7) 0.0408 (4)C4A 0.55440 (7) 0.0338 (3) 0.62590 (7) 0.0470 (s)H5A 0.6100 0.0268 0.6224 $0.056*$ C6A 0.57996 (8) 0.1356 (3) 0.66737 (7) 0.04416 (5)C7A 0.54401 (8) 0.22333 (3) 0.67408 (7) 0.04412 (5)H7A 0.5406 0.2594 0.7024 $0.057*$ C8A 0.51320 (7) 0.2914 (3) 0.63765 (7) 0.04415 (5)H8A 0.58853 -0.0581 0.5110 $0.071*$ C9A 0.59406 (9) -0.0137 (3) 0.54046 (9) 0.0590 (6)H9AA 0.58833 -0.0581 0.5110 $0.071*$ H9AB 0.59377 -0.1007 0.5612 $0.071*$ C1A 0.67930 (11) -0.0200 (5) 0.5770 (11) 0.0882 (10)H11A 0.6738 -0.1102 0.5917 (13) 0.1140 (16)H12A 0.7491 -0.0036 0.6008 $0.143*$ C13A 0.73264 (11) 0.1720 (7) 0.5527 (13) 0.1144 (16)H13A 0.7628 0.2120 0.5592 $0.134*$ C14A 0.69682 (11) 0.2430 (5) 0.5736 (11) $0.078*$ C15A 0.6278 0.2326 0.5031 $0.078*$ C16A 0.4	NZA C1A	0.48818(0) 0.52004(8)	0.3198(2) 0.1662(2)	0.55775(0)	0.0434(4)
CAA $0.4259'(8)$ $0.253'(3)$ $0.3159'(1)$ $0.0305'(5)$ C3A $0.51820'(7)$ $0.2548'(2)$ $0.599'(7)$ $0.0408'(4)$ C4A $0.55440'(7)$ $0.1519'(3)$ $0.58911'(7)$ $0.0423'(4)$ C5A $0.58551'(7)$ $0.0938'(3)$ $0.62590'(7)$ $0.0470'(5)$ H5A 0.6100 0.0268 0.6224 $0.056*$ C6A $0.57996'(8)$ $0.1356'(3)$ $0.6737'(7)$ $0.0481'(5)$ C7A $0.54401'(8)$ $0.2333'(3)$ $0.67408'(7)$ $0.0472'(5)$ H7A 0.5406 $0.2594'$ $0.7024'$ $0.057*'$ C8A $0.51320'(7)$ $0.2914'(3)$ $0.6376'(7)'$ $0.04451'(5)$ H8A 0.4885 $0.3565'$ $0.6416'$ $0.054*'$ C9A $0.59406'(9)$ $-0.0137'(3)$ $0.54046'(9)$ $0.0578'(6)$ C11A $0.67930'(11)$ $-0.0200'(5)$ $0.5757'(11)$ $0.06882'(10)$ H11A $0.6738'$ $-0.1102'$ $0.5917'$ $0.106*'$ C12A $0.72458'(12)$ $0.0428'(8)$ $0.58075'(13)$ $0.1190'(18)$ H12A $0.7491'$ $-0.0036'$ $0.6008'$ $0.143*'$ C13A $0.7628'$ $0.2120''''''''''''''''''''''''''''''''''$	CIA	0.33004 (8)	0.1002(3)	0.30909(7)	0.0524 (6)
CAA 0.51820 (7) 0.2248 (2) 0.53492 (7) 0.0408 (4)C5A 0.5540 (7) 0.0938 (3) 0.62590 (7) 0.0470 (5)H5A 0.6100 0.0268 0.6224 0.056^* C6A 0.57996 (8) 0.1356 (3) 0.6737 (7) 0.04481 (5)C7A 0.54401 (8) 0.2333 (3) 0.67408 (7) 0.0472 (5)H7A 0.5460 0.2594 0.7024 0.057^* C8A 0.51320 (7) 0.2914 (3) 0.63765 (7) 0.04451 (5)H8A 0.4885 0.3565 0.6416 0.0599 (6)H9AA 0.5853 -0.0581 0.5110 0.071^* H9AB 0.5937 -0.1007 0.5612 0.071^* C10A 0.64278 (9) 0.0527 (3) 0.54688 (8) 0.0578 (6)C11A 0.67930 (11) -0.0200 (5) 0.5770 (11) 0.0882 (10)H1A 0.6738 -0.1102 0.5917 0.166^* C12A 0.72458 (12) 0.0428 (8) 0.58075 (13) 0.1190 (18)H12A 0.7491 -0.036 0.6008 0.143^* C13A 0.73264 (11) 0.1720 (7) 0.55272 (13) 0.1114 (16)H13A 0.7626 0.3315 0.5110 0.105^* C15A 0.6278 0.2326 0.5031 0.078^* C15A 0.6278 0.2326 0.5031 0.078^* C15A 0.6278 0.3315 0.5110 0.1054 C15A 0.45048 (8) 0.3578 (3) <td>C2A C2A</td> <td>0.49289 (8)</td> <td>0.2857(5)</td> <td>0.51596 (7)</td> <td>0.0303 (3)</td>	C2A C2A	0.49289 (8)	0.2857(5)	0.51596 (7)	0.0303 (3)
CAA 0.53440 (7) 0.1319 (3) 0.58911 (7) 0.0423 (4)C5A 0.58551 (7) 0.0938 (3) 0.6224 0.056^* C6A 0.57996 (8) 0.1356 (3) 0.66737 (7) 0.0441 (5)C7A 0.54401 (8) 0.2333 (3) 0.67408 (7) 0.0472 (5)T7A 0.5406 0.2594 0.7024 0.057^* C8A 0.51320 (7) 0.2914 (3) 0.63765 (7) 0.04451 (5)H8A 0.48855 0.3565 0.6416 0.0594^* C9A 0.59406 (9) -0.0137 (3) 0.54046 (9) 0.0590 (6)H9AA 0.5853 -0.0581 0.5110 0.071^* H9AB 0.5937 -0.1007 0.5612 0.071^* C10A 0.64278 (9) 0.0527 (3) 0.54688 (8) 0.0578 (6)C11A 0.67390 (11) -0.0200 (5) 0.57570 (11) 0.0682 (10)H11A 0.6738 -0.1102 0.5917 0.106^* C12A 0.72458 (12) 0.0428 (8) 0.58075 (13) 0.1114 (16)H12A 0.7262 0.2120 0.5592 0.134^* C13A 0.73264 (11) 0.1720 (7) 0.55627 (13) 0.1114 (16)H13A 0.7628 0.2120 0.5592 0.134^* C13A 0.73264 (11) 0.1720 (7) 0.5567 (13) 0.1114 (16)H13A 0.7628 0.2120 0.55749 (12) 0.0878 (10)H14A 0.7026 0.3315 0.5110 0.0524 C13A<	C3A	0.51820 (7)	0.2548 (2)	0.59492 (7)	0.0408 (4)
CAA $0.3851 (7)$ $0.0958 (5)$ $0.02290 (7)$ $0.0470 (3)$ H5A 0.6100 0.0268 0.6224 0.056^* C6A $0.57996 (8)$ $0.1356 (3)$ $0.6737 (7)$ $0.0481 (5)$ C7A $0.54401 (8)$ $0.2333 (3)$ $0.67408 (7)$ $0.0472 (5)$ H7A 0.5406 0.2594 0.7024 0.057^* C8A $0.51320 (7)$ $0.2914 (3)$ $0.63765 (7)$ $0.0441 (5)$ H8A 0.4885 0.3565 0.6416 $0.0590 (6)$ H9AA 0.5853 -0.0581 0.5110 0.071^* H9AB 0.5937 -0.1007 0.5612 0.071^* C10A $0.64278 (9)$ $0.0527 (3)$ $0.54688 (8)$ $0.0578 (6)$ C11A $0.67930 (11)$ $-0.200 (5)$ $0.5770 (11)$ $0.1882 (10)$ H11A $0.7326 *$ 0.1102 0.5917 0.106^* C12A $0.72458 (12)$ $0.0428 (8)$ $0.58075 (13)$ $0.1190 (18)$ H12A 0.7491 -0.0036 0.6008 0.143^* C13A $0.73264 (11)$ $0.1200 (5)$ $0.5572 (13)$ $0.114 (16)$ H13A 0.7026 0.3315 0.5110 0.105^* C15A $0.65210 (9)$ $0.1837 (4)$ $0.52278 (9)$ $0.0634 (10)$ H14A 0.7026 $0.3315 (3)$ $0.5503 (10)$ 0.063^* C15A $0.65210 (9)$ $0.1372 (5)$ $0.5011 (0)$ 0.063^* C15A $0.6278 (0)$ $0.3578 (3)$ $0.55367 (8)$ $0.4049 (5)$ C16A <td< td=""><td>C4A</td><td>0.55440 (7)</td><td>0.1519 (3)</td><td>0.58911 (7)</td><td>0.0423 (4)</td></td<>	C4A	0.55440 (7)	0.1519 (3)	0.58911 (7)	0.0423 (4)
HAA 0.6100 0.0268 0.6224 0.056° C6A 0.57996 (8) 0.1356 (3) 0.66737 (7) 0.04481 (5)C7A 0.54401 (8) 0.2333 (3) 0.67408 (7) 0.0472 (5)H7A 0.5406 0.2594 0.7024 0.057^{*} C8A 0.51320 (7) 0.2914 (3) 0.63765 (7) 0.0451 (5)H8A 0.4885 0.3565 0.6416 0.054^{*} C9A 0.59406 (9) -0.0137 (3) 0.54046 (9) 0.0590 (6)H9AA 0.5853 -0.0581 0.5110 0.071^{*} C10A 0.64278 (9) 0.0527 (3) 0.54688 (8) 0.0578 (6)C11A 0.67930 (11) -0.0200 (5) 0.57570 (11) 0.0882 (10)H11A 0.6738 -0.1102 0.5917 0.1106^{*} C12A 0.72458 (12) 0.0428 (8) 0.58075 (13) 0.1190 (18)H12A 0.7491 -0.036 0.6008 0.143^{*} C13A 0.73264 (11) 0.1720 (7) 0.5527 (13) 0.1114 (16)H13A 0.7628 0.2120 0.5917 0.06497 (7)C14A 0.69682 (11) 0.1230 0.5778 (9) 0.06497 (7)H15A 0.65210 (9) 0.8317 (4) 0.52749 (12) 0.0878 (10)H15A 0.6728 0.2326 0.5031 0.078^{*} C16A 0.45048 (8) 0.4351 (3) 0.56138 (8) 0.0524 (5)H16B 0.4572 0.4830 0.59057 (8) 0.0496 (5) <td>C5A</td> <td>0.58551 (/)</td> <td>0.0938 (3)</td> <td>0.62590 (7)</td> <td>0.04/0 (5)</td>	C5A	0.58551 (/)	0.0938 (3)	0.62590 (7)	0.04/0 (5)
CoA 0.57996 (8) 0.1356 (3) 0.66737 (7) 0.0481 (S)C7A 0.54401 (8) 0.2333 (3) 0.67408 (7) 0.0472 (5)H7A 0.5406 0.2294 0.7024 $0.057*$ C8A 0.51320 (7) 0.2914 (3) 0.63765 (7) 0.0451 (5)H8A 0.4885 0.3565 0.6416 $0.054*$ C9A 0.59406 (9) -0.0137 (3) 0.54046 (9) 0.0590 (6)H9AA 0.5853 -0.0581 0.5110 $0.071*$ H9AB 0.5937 -0.1007 0.5612 $0.071*$ C10A 0.64278 (9) 0.0527 (3) 0.54688 (8) 0.0578 (6)C11A 0.67330 (1) -0.0200 (5) 0.57570 (11) 0.0882 (10)H11A 0.6738 -0.1102 0.5917 $0.106*$ C12A 0.72458 (12) 0.4428 (8) 0.58075 (13) 0.1190 (18)H12A 0.7491 -0.0036 0.6008 $0.143*$ C13A 0.7628 0.2120 0.5527 (13) 0.1114 (16)H13A 0.7628 0.2120 0.52749 (12) 0.0878 (10)H14A 0.7026 0.3315 0.5110 $0.105*$ C15A 0.65210 (9) 0.1837 (4) 0.52278 (9) 0.6649 (7)H15A 0.6278 0.2326 0.5031 $0.078*$ C15A 0.4504 (8) 0.4511 (3) 0.5905 $0.663*$ C15A 0.4504 (8) 0.45151 (3) 0.5905 $0.663*$ C15A 0.4502 0.5208 <td>H5A</td> <td>0.6100</td> <td>0.0268</td> <td>0.6224</td> <td>0.056*</td>	H5A	0.6100	0.0268	0.6224	0.056*
C/A 0.54401 (8) 0.2333 (3) 0.67408 (7) 0.0472 (s)H7A 0.5406 0.2594 0.7024 $0.057*$ C8A 0.51320 (7) 0.2914 (3) 0.63765 (7) 0.04451 (5)H8A 0.4885 0.3565 0.6416 $0.054*$ C9A 0.59406 (9) -0.0137 (3) 0.54046 (9) 0.0590 (6)H9AA 0.5853 -0.0581 0.5110 $0.071*$ H9AB 0.5937 -0.1007 0.5612 $0.071*$ C10A 0.64278 (9) 0.0527 (3) 0.54648 (8) 0.0578 (6)C11A 0.67930 (11) -0.0200 (5) 0.57570 (11) 0.0882 (10)H11A 0.6738 -0.1102 0.5917 $0.106*$ C12A 0.72458 (12) 0.0428 (8) 0.58075 (13) 0.1190 (18)H12A 0.7741 -0.0036 0.6008 $0.143*$ C13A 0.73264 (11) 0.1720 (7) 0.55627 (13) 0.1114 (16)H13A 0.7628 0.2120 0.5592 $0.134*$ C14A 0.69682 (11) 0.2430 (5) 0.52749 (12) 0.0878 (10)H14A 0.7026 0.3315 0.5110 $0.105*$ C15A 0.65210 (9) 0.1837 (4) 0.52278 (9) 0.0649 (7)H15A 0.6778 0.2326 0.5031 $0.078*$ C16A 0.45048 (8) 0.4551 (3) 0.5905 $0.663*$ C15A 0.4502 0.5208 0.5401 $0.063*$ C15A 0.32639 (10) 0.335	C6A	0.57996 (8)	0.1356 (3)	0.66737(7)	0.0481 (5)
$H7A$ 0.5406 0.22944 0.7024 0.057^* $C8A$ 0.51320 (7) 0.2914 (3) 0.63765 (7) 0.0451 (5) $H8A$ 0.4885 0.3565 0.6416 $0.054*$ $C9A$ 0.59406 (9) -0.0137 (3) 0.54046 (9) 0.0590 (6) $H9AA$ 0.5853 -0.0581 0.5110 $0.071*$ $L9AA$ 0.64278 (9) 0.0527 (3) 0.54688 (8) 0.0578 (6) $C11A$ 0.67930 (1) -0.0200 (5) 0.57570 (1) 0.0882 (10) $H11A$ 0.6738 -0.1102 0.5917 0.106^* $C12A$ 0.72458 (12) 0.0428 (8) 0.58075 (13) 0.1190 (18) $H12A$ 0.7491 -0.0036 0.6008 0.143^* $C13A$ 0.73264 (11) 0.1720 (7) 0.55627 (13) 0.1114 (16) $H13A$ 0.66982 (11) 0.2430 (5) 0.52749 (12) 0.0878 (10) $H14A$ 0.7026 0.3315 0.5110 0.105^* $C15A$ 0.65210 (9) 0.1837 (4) 0.52278 (9) 0.0649 (7) $H15A$ 0.6278 0.2326 0.5031 0.078^* $C15A$ 0.45048 (8) 0.4351 (3) 0.56138 (8) 0.0524 (5) $H16B$ 0.4502 0.5208 0.5401 0.063^* $H16B$ 0.4502 0.33578 (3) 0.55367 (8) 0.0496 (5) $C17A$ 0.40279 (8) 0.3578 (3) 0.55367 (8) 0.0496 (5) $C18A$ 0.37076 (10) 0.3351 (4) 0.5199 (C/A	0.54401 (8)	0.2333 (3)	0.67408 (7)	0.04/2 (5)
C8A 0.51320 (7) 0.2914 (3) 0.63765 (7) 0.0451 (5) H8A 0.4885 0.3565 0.6416 0.0594 C9A 0.59406 (9) -0.0137 (3) 0.54046 (9) 0.0590 (6) H9AA 0.5853 -0.0581 0.5110 0.071* H9AB 0.5937 -0.1007 0.5612 0.071* C10A 0.64278 (9) 0.0527 (3) 0.54688 (8) 0.0578 (6) C11A 0.67930 (11) -0.0200 (5) 0.57570 (11) 0.0882 (10) H11A 0.6738 -0.1102 0.5917 0.106* C12A 0.72458 (12) 0.0428 (8) 0.58075 (13) 0.1190 (18) H12A 0.7491 -0.0036 0.6008 0.143* C13A 0.72628 0.2120 0.5592 0.134* C14A 0.69682 (11) 0.2430 (5) 0.52749 (12) 0.0878 (10) H14A 0.7026 0.3315 0.5110 0.105* C15A 0.65210 (9) 0.1837 (4) 0.52278 (9) 0.0649 (7) <td>H7A</td> <td>0.5406</td> <td>0.2594</td> <td>0.7024</td> <td>0.057*</td>	H7A	0.5406	0.2594	0.7024	0.057*
H8A 0.4885 0.3565 0.6416 0.054* C9A 0.59406 (9) -0.0137 (3) 0.54046 (9) 0.0590 (6) H9AA 0.5853 -0.0581 0.5110 0.071* H9AB 0.5937 -0.1007 0.5612 0.071* C10A 0.64278 (9) 0.0527 (3) 0.54688 (8) 0.0578 (6) C11A 0.67930 (11) -0.0200 (5) 0.57570 (11) 0.0828 (10) H1A 0.6738 -0.1102 0.5917 0.106* C12A 0.72458 (12) 0.0428 (8) 0.58075 (13) 0.1114 (16) H1A 0.6738 -0.1102 0.55627 (13) 0.1114 (16) H13A 0.7628 0.2120 0.5592 0.134* C14A 0.69682 (11) 0.2430 (5) 0.52749 (12) 0.0878 (10) H14A 0.7026 0.3315 0.5110 0.105* C15A 0.65210 (9) 0.1837 (4) 0.52278 (9) 0.6643 (7) H15A 0.6278 0.2326 0.5301 0.078* </td <td>C8A</td> <td>0.51320 (7)</td> <td>0.2914 (3)</td> <td>0.63765 (7)</td> <td>0.0451 (5)</td>	C8A	0.51320 (7)	0.2914 (3)	0.63765 (7)	0.0451 (5)
C9A 0.59406 (9) -0.0137 (3) 0.54046 (9) 0.0590 (6) H9AA 0.5853 -0.0581 0.5110 0.071* H9AB 0.5937 -0.1007 0.5612 0.071* C10A 0.64278 (9) 0.0527 (3) 0.54688 (8) 0.0578 (6) C11A 0.67930 (11) -0.0200 (5) 0.57570 (11) 0.0882 (10) H11A 0.6738 -0.1102 0.5917 0.106* C12A 0.72458 (12) 0.0428 (8) 0.58075 (13) 0.1190 (18) H12A 0.7491 -0.0036 0.6008 0.143* C13A 0.73264 (11) 0.1720 (7) 0.55627 (13) 0.1114 (16) H13A 0.7628 0.2120 0.5572 0.134* C15A 0.69682 (11) 0.2430 (5) 0.5278 (9) 0.0649 (7) H14A 0.7026 0.3315 0.5110 0.105* C15A 0.65210 (9) 0.1837 (4) 0.5278 (9) 0.0649 (7) H15A 0.6278 0.2326 0.5031 0.078* <td>H8A</td> <td>0.4885</td> <td>0.3565</td> <td>0.6416</td> <td>0.054*</td>	H8A	0.4885	0.3565	0.6416	0.054*
H9AA 0.5853 -0.0581 0.5110 0.071* H9AB 0.5937 -0.1007 0.5612 0.071* C10A 0.64278 (9) 0.0527 (3) 0.54688 (8) 0.0578 (6) C11A 0.67930 (11) -0.0200 (5) 0.57570 (11) 0.0882 (10) H11A 0.6738 -0.1102 0.5917 0.106* C12A 0.72458 (12) 0.0428 (8) 0.58075 (13) 0.1190 (18) H12A 0.7491 -0.0036 0.6008 0.143* C13A 0.73264 (11) 0.1720 (7) 0.55627 (13) 0.1114 (16) H13A 0.7628 0.2120 0.5592 0.134* C14A 0.69682 (11) 0.2430 (5) 0.52749 (12) 0.0878 (10) H14A 0.7026 0.3315 0.5110 0.105* C15A 0.65210 (9) 0.1837 (4) 0.52278 (9) 0.0649 (7) H15A 0.6278 0.2326 0.5031 0.078* C16A 0.4502 0.5208 0.5401 0.063*	C9A	0.59406 (9)	-0.0137 (3)	0.54046 (9)	0.0590 (6)
H9AB 0.5937 -0.1007 0.5612 0.071* C10A 0.64278 (9) 0.0527 (3) 0.54688 (8) 0.0578 (6) C11A 0.67930 (11) -0.0200 (5) 0.57570 (11) 0.0882 (10) H11A 0.6738 -0.1102 0.5917 0.106* C12A 0.72458 (12) 0.0428 (8) 0.58075 (13) 0.1190 (18) H12A 0.7491 -0.0036 0.6008 0.143* C13A 0.73264 (11) 0.1720 (7) 0.55627 (13) 0.1114 (16) H13A 0.7628 0.2120 0.5592 0.134* C14A 0.69682 (11) 0.2430 (5) 0.52749 (12) 0.0878 (10) H14A 0.7026 0.3315 0.5110 0.105* C15A 0.65210 (9) 0.1837 (4) 0.52278 (9) 0.0649 (7) H15A 0.6278 0.2326 0.5031 0.078* C16A 0.45048 (8) 0.4351 (3) 0.56138 (8) 0.0524 (5) H16B 0.4572 0.4830 0.5905 0.063*	H9AA	0.5853	-0.0581	0.5110	0.071*
C10A 0.64278 (9) 0.0527 (3) 0.54688 (8) 0.0578 (6)C11A 0.67930 (11) -0.0200 (5) 0.57570 (11) 0.0882 (10)H11A 0.6738 -0.1102 0.5917 $0.106*$ C12A 0.72458 (12) 0.0428 (8) 0.58075 (13) 0.1190 (18)H12A 0.7491 -0.0036 0.6008 $0.143*$ C13A 0.73264 (11) 0.1720 (7) 0.55627 (13) 0.1114 (16)H13A 0.7628 0.2120 0.5592 $0.134*$ C14A 0.69682 (11) 0.2430 (5) 0.52749 (12) 0.0878 (10)H14A 0.7026 0.3315 0.5110 $0.105*$ C15A 0.65210 (9) 0.1837 (4) 0.52278 (9) 0.0649 (7)H15A 0.6278 0.2326 0.5031 $0.078*$ C16A 0.45048 (8) 0.4351 (3) 0.56138 (8) 0.0524 (5)H16A 0.4502 0.5208 0.5401 $0.063*$ H16B 0.4572 0.4830 0.5905 $0.063*$ C17A 0.40279 (8) 0.3578 (3) 0.55367 (8) 0.0496 (5)C18A 0.3706 (10) 0.3851 (4) 0.51459 (9) 0.0653 (7)H18A 0.3700 0.4489 0.4928 $0.078*$ C19A 0.32639 (10) 0.3172 (5) 0.50810 (11) 0.0825 (9)H19A 0.3051 0.3363 0.4819 $0.099*$ C20A 0.31370 (10) 0.2231 (4) 0.53952 (13) 0.0851 (10)H20A <t< td=""><td>H9AB</td><td>0.5937</td><td>-0.1007</td><td>0.5612</td><td>0.071*</td></t<>	H9AB	0.5937	-0.1007	0.5612	0.071*
C11A 0.67930 (11) -0.0200 (5) 0.57570 (11) 0.0882 (10) H11A 0.6738 -0.1102 0.5917 0.106* C12A 0.72458 (12) 0.0428 (8) 0.58075 (13) 0.1190 (18) H12A 0.7491 -0.0036 0.6008 0.143* C13A 0.73264 (11) 0.1720 (7) 0.55627 (13) 0.1114 (16) H13A 0.7628 0.2120 0.5592 0.134* C14A 0.69682 (11) 0.2430 (5) 0.52749 (12) 0.0649 (7) H14A 0.7026 0.3315 0.5110 0.105* C15A 0.65210 (9) 0.1837 (4) 0.52278 (9) 0.0649 (7) H15A 0.6278 0.2326 0.5031 0.078* C16A 0.45048 (8) 0.4351 (3) 0.56138 (8) 0.0524 (5) H16B 0.4572 0.4830 0.5905 0.063* C17A 0.40279 (8) 0.3578 (3) 0.55367 (8) 0.0496 (5) C18A 0.37076 (10) 0.3814 (4) 0.51459 (9)	C10A	0.64278 (9)	0.0527 (3)	0.54688 (8)	0.0578 (6)
H11A 0.6738 -0.1102 0.5917 $0.106*$ C12A $0.72458(12)$ $0.0428(8)$ $0.58075(13)$ $0.1190(18)$ H12A 0.7491 -0.0036 0.6008 $0.143*$ C13A $0.73264(11)$ $0.1720(7)$ $0.55627(13)$ $0.1114(16)$ H13A 0.7628 0.2120 0.5592 $0.134*$ C14A $0.69682(11)$ $0.2430(5)$ $0.52749(12)$ $0.0878(10)$ H14A 0.7026 0.3315 0.5110 $0.105*$ C15A $0.65210(9)$ $0.1837(4)$ $0.52278(9)$ $0.0649(7)$ H15A 0.6278 0.2326 0.5031 $0.078*$ C16A $0.45048(8)$ $0.4351(3)$ $0.56138(8)$ $0.0524(5)$ H16A 0.4502 0.5208 0.5401 $0.063*$ C17A $0.4279(8)$ $0.3578(3)$ $0.55367(8)$ $0.0496(5)$ C18A $0.37076(10)$ $0.3851(4)$ $0.51459(9)$ $0.0653(7)$ H18A 0.3707 0.3363 0.4819 $0.999*$ C19A $0.32639(10)$ $0.3172(5)$ $0.50810(11)$ $0.0825(9)$ H19A 0.3051 0.3363 0.4819 $0.099*$ C20A $0.31370(10)$ $0.2231(4)$ $0.5739(13)$ $0.0851(10)$ H20A 0.2840 0.1773 0.5347 $0.102*$ C21A $0.3492(1)$ 0.1335 0.6002 $0.103*$ C22A $0.38924(9)$ $0.2617(4)$ $0.58501(10)$ $0.0679(7)$ H22A 0.4104 0.2407 0.6112 0.081	C11A	0.67930 (11)	-0.0200(5)	0.57570 (11)	0.0882 (10)
C12A 0.72458 (12) 0.0428 (8) 0.58075 (13) 0.1190 (18) H12A 0.7491 -0.0036 0.6008 0.143* C13A 0.73264 (11) 0.1720 (7) 0.55627 (13) 0.1114 (16) H13A 0.7628 0.2120 0.5592 0.134* C14A 0.69682 (11) 0.2430 (5) 0.52749 (12) 0.0878 (10) H14A 0.7026 0.3315 0.5110 0.105* C15A 0.65210 (9) 0.1837 (4) 0.52278 (9) 0.0649 (7) H15A 0.6278 0.2326 0.5031 0.078* C16A 0.45048 (8) 0.4351 (3) 0.56138 (8) 0.0524 (5) H16A 0.4502 0.5208 0.5401 0.663* C17A 0.40279 (8) 0.3578 (3) 0.551367 (8) 0.0496 (5) C18A 0.37076 (10) 0.3851 (4) 0.51459 (9) 0.6653 (7) H18A 0.3700 0.4489 0.4928 0.078* C19A 0.32639 (10) 0.3172 (5) 0.50810 (11)	H11A	0.6738	-0.1102	0.5917	0.106*
H12A0.7491-0.00360.60080.143*C13A0.73264 (11)0.1720 (7)0.55627 (13)0.1114 (16)H13A0.76280.21200.55920.134*C14A0.69682 (11)0.2430 (5)0.52749 (12)0.0878 (10)H14A0.70260.33150.51100.105*C15A0.65210 (9)0.1837 (4)0.52278 (9)0.0649 (7)H15A0.62780.23260.50310.078*C16A0.45048 (8)0.4351 (3)0.56138 (8)0.0524 (5)H16A0.45020.52080.54010.063*H16B0.45720.48300.59050.063*C17A0.40279 (8)0.3578 (3)0.55367 (8)0.0496 (5)C18A0.37076 (10)0.3851 (4)0.51459 (9)0.0653 (7)H18A0.37000.44890.49280.078*C19A0.32639 (10)0.3172 (5)0.50810 (11)0.0825 (9)H19A0.30510.33630.48190.099*C20A0.31370 (10)0.2231 (4)0.53952 (13)0.0851 (10)H20A0.28400.17730.53470.102*C21A0.34496 (11)0.1960 (4)0.5739 (13)0.0856 (10)H21A0.33630.42070.61120.081*C22A0.38924 (9)0.2617 (4)0.58501 (10)0.0679 (7)H22A0.41040.24070.61120.081*	C12A	0.72458 (12)	0.0428 (8)	0.58075 (13)	0.1190 (18)
C13A0.73264 (11)0.1720 (7)0.55627 (13)0.1114 (16)H13A0.76280.21200.55920.134*C14A0.69682 (11)0.2430 (5)0.52749 (12)0.0878 (10)H14A0.70260.33150.51100.105*C15A0.65210 (9)0.1837 (4)0.52278 (9)0.0649 (7)H15A0.62780.23260.50310.078*C16A0.45048 (8)0.4351 (3)0.56138 (8)0.0524 (5)H16A0.45020.52080.54010.063*H16B0.45720.48300.59050.063*C17A0.40279 (8)0.3578 (3)0.55367 (8)0.0496 (5)C18A0.37076 (10)0.3851 (4)0.51459 (9)0.0653 (7)H18A0.37900.44890.49280.078*C19A0.32639 (10)0.3172 (5)0.50810 (11)0.0825 (9)H19A0.30510.33630.48190.099*C20A0.3170 (10)0.2231 (4)0.53952 (13)0.0851 (10)H20A0.28400.17730.53470.102*C21A0.34496 (11)0.1960 (4)0.57839 (13)0.0856 (10)H21A0.33630.13350.60020.103*C22A0.38924 (9)0.2617 (4)0.58501 (10)0.0679 (7)H22A0.41040.24070.61120.081*C11B0.33081 (3)0.58144 (10)0.37621 (3)0.0797 (2)	H12A	0.7491	-0.0036	0.6008	0.143*
H13A0.76280.21200.55920.134*C14A0.69682 (11)0.2430 (5)0.52749 (12)0.0878 (10)H14A0.70260.33150.51100.105*C15A0.65210 (9)0.1837 (4)0.52278 (9)0.0649 (7)H15A0.62780.23260.50310.078*C16A0.45048 (8)0.4351 (3)0.56138 (8)0.0524 (5)H16A0.45020.52080.54010.063*H16B0.45720.48300.59050.063*C17A0.40279 (8)0.3578 (3)0.55367 (8)0.0496 (5)C18A0.37076 (10)0.3851 (4)0.51459 (9)0.0653 (7)H18A0.37900.44890.49280.078*C19A0.32639 (10)0.3172 (5)0.5010 (11)0.0825 (9)H19A0.30510.33630.48190.099*C20A0.31370 (10)0.2231 (4)0.53952 (13)0.0851 (10)H20A0.28400.17730.53470.102*C21A0.34496 (11)0.1960 (4)0.57839 (13)0.0856 (10)H21A0.33630.13350.60020.103*C22A0.38924 (9)0.2617 (4)0.58501 (10)0.0679 (7)H22A0.41040.24070.61120.081*C11B0.33081 (3)0.58144 (10)0.37621 (3)0.0797 (2)	C13A	0.73264 (11)	0.1720 (7)	0.55627 (13)	0.1114 (16)
C14A0.69682 (11)0.2430 (5)0.52749 (12)0.0878 (10)H14A0.70260.33150.51100.105*C15A0.65210 (9)0.1837 (4)0.52278 (9)0.0649 (7)H15A0.62780.23260.50310.078*C16A0.45048 (8)0.4351 (3)0.56138 (8)0.0524 (5)H16A0.45020.52080.54010.063*H16B0.45720.48300.59050.063*C17A0.40279 (8)0.3578 (3)0.51459 (9)0.0653 (7)H18A0.37076 (10)0.3851 (4)0.51459 (9)0.0653 (7)H18A0.37900.44890.49280.078*C19A0.32639 (10)0.3172 (5)0.50810 (11)0.0825 (9)H19A0.30510.33630.48190.099*C20A0.31370 (10)0.2231 (4)0.53952 (13)0.0851 (10)H20A0.28400.17730.53470.102*C21A0.34496 (11)0.1960 (4)0.57839 (13)0.0856 (10)H21A0.33630.13350.60020.103*C22A0.38924 (9)0.2617 (4)0.58501 (10)0.0679 (7)H22A0.41040.24070.61120.081*C11B0.33081 (3)0.58144 (10)0.37621 (3)0.0797 (2)	H13A	0.7628	0.2120	0.5592	0.134*
H14A0.70260.33150.51100.105*C15A0.65210 (9)0.1837 (4)0.52278 (9)0.0649 (7)H15A0.62780.23260.50310.078*C16A0.45048 (8)0.4351 (3)0.56138 (8)0.0524 (5)H16A0.45020.52080.54010.063*H16B0.45720.48300.59050.063*C17A0.40279 (8)0.3578 (3)0.55367 (8)0.0496 (5)C18A0.37076 (10)0.3851 (4)0.51459 (9)0.0653 (7)H18A0.37900.44890.49280.078*C19A0.32639 (10)0.3172 (5)0.50810 (11)0.0825 (9)H19A0.30510.33630.48190.099*C20A0.31370 (10)0.2231 (4)0.53952 (13)0.0851 (10)H20A0.28400.17730.53470.102*C21A0.3496 (11)0.1960 (4)0.57839 (13)0.0856 (10)H21A0.33630.13350.60020.103*C22A0.38924 (9)0.2617 (4)0.58501 (10)0.0679 (7)H22A0.41040.24070.61120.081*C11B0.33081 (3)0.58144 (10)0.37621 (3)0.0797 (2)	C14A	0.69682 (11)	0.2430 (5)	0.52749 (12)	0.0878 (10)
C15A0.65210 (9)0.1837 (4)0.52278 (9)0.0649 (7)H15A0.62780.23260.50310.078*C16A0.45048 (8)0.4351 (3)0.56138 (8)0.0524 (5)H16A0.45020.52080.54010.063*H16B0.45720.48300.59050.063*C17A0.40279 (8)0.3578 (3)0.55367 (8)0.0496 (5)C18A0.37076 (10)0.3851 (4)0.51459 (9)0.0653 (7)H18A0.37900.44890.49280.078*C19A0.32639 (10)0.3172 (5)0.50810 (11)0.0825 (9)H19A0.30510.33630.48190.099*C20A0.31370 (10)0.2231 (4)0.53952 (13)0.0851 (10)H20A0.28400.17730.53470.102*C21A0.3496 (11)0.1960 (4)0.57839 (13)0.0856 (10)H21A0.33630.13350.60020.103*C22A0.38924 (9)0.2617 (4)0.58501 (10)0.0679 (7)H22A0.41040.24070.61120.081*C11B0.33081 (3)0.58144 (10)0.37621 (3)0.0797 (2)	H14A	0.7026	0.3315	0.5110	0.105*
H15A0.62780.23260.50310.078*C16A0.45048 (8)0.4351 (3)0.56138 (8)0.0524 (5)H16A0.45020.52080.54010.063*H16B0.45720.48300.59050.063*C17A0.40279 (8)0.3578 (3)0.55367 (8)0.0496 (5)C18A0.37076 (10)0.3851 (4)0.51459 (9)0.0653 (7)H18A0.37090.44890.49280.078*C19A0.32639 (10)0.3172 (5)0.50810 (11)0.0825 (9)H19A0.30510.33630.48190.099*C20A0.31370 (10)0.2231 (4)0.53952 (13)0.0851 (10)H20A0.28400.17730.53470.102*C21A0.34496 (11)0.1960 (4)0.57839 (13)0.0856 (10)H21A0.33630.13350.60020.103*C22A0.38924 (9)0.2617 (4)0.58501 (10)0.0679 (7)H22A0.41040.24070.61120.081*C11B0.33081 (3)0.58144 (10)0.37621 (3)0.0797 (2)	C15A	0.65210 (9)	0.1837 (4)	0.52278 (9)	0.0649 (7)
C16A0.45048 (8)0.4351 (3)0.56138 (8)0.0524 (5)H16A0.45020.52080.54010.063*H16B0.45720.48300.59050.063*C17A0.40279 (8)0.3578 (3)0.55367 (8)0.0496 (5)C18A0.37076 (10)0.3851 (4)0.51459 (9)0.0653 (7)H18A0.37900.44890.49280.078*C19A0.32639 (10)0.3172 (5)0.50810 (11)0.0825 (9)H19A0.30510.33630.48190.099*C20A0.31370 (10)0.2231 (4)0.53952 (13)0.0851 (10)H20A0.28400.17730.53470.102*C21A0.34496 (11)0.1960 (4)0.57839 (13)0.0856 (10)H21A0.33630.13350.60020.103*C22A0.38924 (9)0.2617 (4)0.58501 (10)0.0679 (7)H22A0.41040.24070.61120.081*C11B0.33081 (3)0.58144 (10)0.37621 (3)0.0797 (2)	H15A	0.6278	0.2326	0.5031	0.078*
H16A0.45020.52080.54010.063*H16B0.45720.48300.59050.063*C17A0.40279 (8)0.3578 (3)0.55367 (8)0.0496 (5)C18A0.37076 (10)0.3851 (4)0.51459 (9)0.0653 (7)H18A0.37900.44890.49280.078*C19A0.32639 (10)0.3172 (5)0.50810 (11)0.0825 (9)H19A0.30510.33630.48190.099*C20A0.31370 (10)0.2231 (4)0.53952 (13)0.0851 (10)H20A0.28400.17730.53470.102*C21A0.34496 (11)0.1960 (4)0.57839 (13)0.0856 (10)H21A0.33630.13350.60020.103*C22A0.38924 (9)0.2617 (4)0.58501 (10)0.0679 (7)H22A0.41040.24070.61120.081*C11B0.33081 (3)0.58144 (10)0.37621 (3)0.0797 (2)	C16A	0.45048 (8)	0.4351 (3)	0.56138 (8)	0.0524 (5)
H16B0.45720.48300.59050.063*C17A0.40279 (8)0.3578 (3)0.55367 (8)0.0496 (5)C18A0.37076 (10)0.3851 (4)0.51459 (9)0.0653 (7)H18A0.37900.44890.49280.078*C19A0.32639 (10)0.3172 (5)0.50810 (11)0.0825 (9)H19A0.30510.33630.48190.099*C20A0.31370 (10)0.2231 (4)0.53952 (13)0.0851 (10)H20A0.28400.17730.53470.102*C21A0.34496 (11)0.1960 (4)0.57839 (13)0.0856 (10)H21A0.33630.13350.60020.103*C22A0.38924 (9)0.2617 (4)0.58501 (10)0.0679 (7)H22A0.41040.24070.61120.081*C11B0.33081 (3)0.58144 (10)0.37621 (3)0.0797 (2)	H16A	0.4502	0.5208	0.5401	0.063*
C17A0.40279 (8)0.3578 (3)0.55367 (8)0.0496 (5)C18A0.37076 (10)0.3851 (4)0.51459 (9)0.0653 (7)H18A0.37900.44890.49280.078*C19A0.32639 (10)0.3172 (5)0.50810 (11)0.0825 (9)H19A0.30510.33630.48190.099*C20A0.31370 (10)0.2231 (4)0.53952 (13)0.0851 (10)H20A0.28400.17730.53470.102*C21A0.34496 (11)0.1960 (4)0.57839 (13)0.0856 (10)H21A0.33630.13350.60020.103*C22A0.38924 (9)0.2617 (4)0.58501 (10)0.0679 (7)H22A0.41040.24070.61120.081*C11B0.33081 (3)0.58144 (10)0.37621 (3)0.0797 (2)	H16B	0.4572	0.4830	0.5905	0.063*
C18A0.37076 (10)0.3851 (4)0.51459 (9)0.0653 (7)H18A0.37900.44890.49280.078*C19A0.32639 (10)0.3172 (5)0.50810 (11)0.0825 (9)H19A0.30510.33630.48190.099*C20A0.31370 (10)0.2231 (4)0.53952 (13)0.0851 (10)H20A0.28400.17730.53470.102*C21A0.34496 (11)0.1960 (4)0.57839 (13)0.0856 (10)H21A0.33630.13350.60020.103*C22A0.38924 (9)0.2617 (4)0.58501 (10)0.0679 (7)H22A0.41040.24070.61120.081*C11B0.33081 (3)0.58144 (10)0.37621 (3)0.0797 (2)	C17A	0.40279 (8)	0.3578 (3)	0.55367 (8)	0.0496 (5)
H18A0.37900.44890.49280.078*C19A0.32639 (10)0.3172 (5)0.50810 (11)0.0825 (9)H19A0.30510.33630.48190.099*C20A0.31370 (10)0.2231 (4)0.53952 (13)0.0851 (10)H20A0.28400.17730.53470.102*C21A0.34496 (11)0.1960 (4)0.57839 (13)0.0856 (10)H21A0.33630.13350.60020.103*C22A0.38924 (9)0.2617 (4)0.58501 (10)0.0679 (7)H22A0.41040.24070.61120.081*C11B0.33081 (3)0.58144 (10)0.37621 (3)0.0797 (2)	C18A	0.37076 (10)	0.3851 (4)	0.51459 (9)	0.0653 (7)
C19A0.32639 (10)0.3172 (5)0.50810 (11)0.0825 (9)H19A0.30510.33630.48190.099*C20A0.31370 (10)0.2231 (4)0.53952 (13)0.0851 (10)H20A0.28400.17730.53470.102*C21A0.34496 (11)0.1960 (4)0.57839 (13)0.0856 (10)H21A0.33630.13350.60020.103*C22A0.38924 (9)0.2617 (4)0.58501 (10)0.0679 (7)H22A0.41040.24070.61120.081*C11B0.33081 (3)0.58144 (10)0.37621 (3)0.0797 (2)	H18A	0.3790	0.4489	0.4928	0.078*
H19A0.30510.33630.48190.099*C20A0.31370 (10)0.2231 (4)0.53952 (13)0.0851 (10)H20A0.28400.17730.53470.102*C21A0.34496 (11)0.1960 (4)0.57839 (13)0.0856 (10)H21A0.33630.13350.60020.103*C22A0.38924 (9)0.2617 (4)0.58501 (10)0.0679 (7)H22A0.41040.24070.61120.081*C11B0.33081 (3)0.58144 (10)0.37621 (3)0.0797 (2)	C19A	0.32639 (10)	0.3172 (5)	0.50810 (11)	0.0825 (9)
C20A0.31370 (10)0.2231 (4)0.53952 (13)0.0851 (10)H20A0.28400.17730.53470.102*C21A0.34496 (11)0.1960 (4)0.57839 (13)0.0856 (10)H21A0.33630.13350.60020.103*C22A0.38924 (9)0.2617 (4)0.58501 (10)0.0679 (7)H22A0.41040.24070.61120.081*C11B0.33081 (3)0.58144 (10)0.37621 (3)0.0797 (2)	H19A	0.3051	0.3363	0.4819	0.099*
H20A0.28400.17730.53470.102*C21A0.34496 (11)0.1960 (4)0.57839 (13)0.0856 (10)H21A0.33630.13350.60020.103*C22A0.38924 (9)0.2617 (4)0.58501 (10)0.0679 (7)H22A0.41040.24070.61120.081*C11B0.33081 (3)0.58144 (10)0.37621 (3)0.0797 (2)	C20A	0.31370 (10)	0.2231 (4)	0.53952 (13)	0.0851 (10)
C21A0.34496 (11)0.1960 (4)0.57839 (13)0.0856 (10)H21A0.33630.13350.60020.103*C22A0.38924 (9)0.2617 (4)0.58501 (10)0.0679 (7)H22A0.41040.24070.61120.081*C11B0.33081 (3)0.58144 (10)0.37621 (3)0.0797 (2)	H20A	0.2840	0.1773	0.5347	0.102*
H21A0.33630.13350.60020.103*C22A0.38924 (9)0.2617 (4)0.58501 (10)0.0679 (7)H22A0.41040.24070.61120.081*C11B0.33081 (3)0.58144 (10)0.37621 (3)0.0797 (2)	C21A	0.34496 (11)	0.1960 (4)	0.57839 (13)	0.0856 (10)
C22A0.38924 (9)0.2617 (4)0.58501 (10)0.0679 (7)H22A0.41040.24070.61120.081*C11B0.33081 (3)0.58144 (10)0.37621 (3)0.0797 (2)	H21A	0.3363	0.1335	0.6002	0.103*
H22A0.41040.24070.61120.081*C11B0.33081 (3)0.58144 (10)0.37621 (3)0.0797 (2)	C22A	0.38924 (9)	0.2617 (4)	0.58501 (10)	0.0679 (7)
Cl1B 0.33081 (3) 0.58144 (10) 0.37621 (3) 0.0797 (2)	H22A	0.4104	0.2407	0.6112	0.081*
	Cl1B	0.33081 (3)	0.58144 (10)	0.37621 (3)	0.0797 (2)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\hat{A}^2)

O1B	0.43598 (6)	0.2708 (2)	0.19629 (5)	0.0610 (5)
O2B	0.49943 (6)	0.0979 (2)	0.25341 (6)	0.0627 (4)
N1B	0.40704 (6)	0.3788 (2)	0.25221 (5)	0.0427 (4)
N2B	0.47554 (6)	0.2118 (2)	0.31145 (6)	0.0429 (4)
C1B	0.43687 (7)	0.2823 (3)	0.23545 (7)	0.0445 (5)
C2B	0.47303 (7)	0.1879 (3)	0.26761 (7)	0.0457 (5)
C3B	0.44279 (7)	0.3067 (2)	0.32762 (6)	0.0405 (4)
C4B	0.40761 (7)	0.3855 (3)	0.29761 (6)	0.0401 (4)
C5B	0.37306 (7)	0.4698 (3)	0.31310 (7)	0.0468 (5)
H5B	0.3489	0.5198	0.2935	0.056*
C6B	0.37493 (9)	0.4785 (3)	0.35796 (8)	0.0534 (6)
C7B	0.41028 (9)	0.4089 (3)	0.38768 (7)	0.0537 (6)
H7B	0.4115	0.4190	0.4177	0.064*
C8B	0.44431 (8)	0.3231 (3)	0.37248 (7)	0.0484 (5)
H8B	0.4686	0.2756	0.3926	0.058*
C9B	0.37628 (8)	0.4870 (3)	0.22173 (7)	0.0530 (5)
H9BA	0.3877	0.4937	0.1946	0.064*
H9BB	0.3782	0.5939	0.2345	0.064*
C10B	0.32551 (8)	0.4356 (3)	0.21095 (7)	0.0543 (6)
C11B	0.31232 (10)	0.2785 (4)	0.20404 (11)	0.0754 (8)
H11B	0.3351	0.1991	0.2062	0.091*
C12B	0.26533 (12)	0.2348 (5)	0.19378 (12)	0.0946 (11)
H12B	0.2570	0.1271	0.1893	0.113*
C13B	0.23174 (11)	0.3487 (7)	0.19036 (12)	0.1002 (13)
H13B	0.2003	0.3196	0.1837	0.120*
C14B	0.24408 (12)	0.5056 (7)	0.19666 (14)	0.1053 (13)
H14B	0.2210	0.5842	0.1939	0.126*
C15B	0.29074 (11)	0.5500 (5)	0.20722 (12)	0.0840 (9)
H15B	0.2987	0.6580	0.2118	0.101*
C16B	0.51314 (7)	0.1264 (3)	0.34172 (8)	0.0487 (5)
H16C	0.5194	0.0257	0.3282	0.058*
H16D	0.5024	0.1007	0.3685	0.058*
C17B	0.55802 (7)	0.2199 (3)	0.35376 (7)	0.0421 (4)
C18B	0.59036 (9)	0.1716 (4)	0.39071 (8)	0.0608 (6)
H18B	0.5827	0.0906	0.4086	0.073*
C19B	0.63370 (9)	0.2428 (4)	0.40097 (10)	0.0765 (9)
H19B	0.6553	0.2084	0.4256	0.092*
C20B	0.64540 (10)	0.3633 (4)	0.37538 (11)	0.0771 (8)
H20B	0.6750	0.4098	0.3822	0.093*
C21B	0.61317 (10)	0.4150 (4)	0.33963 (11)	0.0752 (8)
H21B	0.6208	0.4987	0.3225	0.090*
C22B	0.56949 (9)	0.3443 (3)	0.32867 (9)	0.0597 (6)
H22B	0.5479	0.3808	0.3043	0.072*

Atomic displacement parameters $(Å^2)$

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	<i>U</i> ²³
Cl1A	0.0533 (3)	0.0909 (5)	0.0550 (3)	-0.0014 (3)	0.0025 (2)	0.0022 (3)

01A	0.0727 (12)	0.1090 (16)	0.0461 (9)	-0.0143 (11)	0.0256 (8)	-0.0145 (10)
O2A	0.0555 (10)	0.0907 (13)	0.0486 (9)	-0.0118 (9)	0.0072 (7)	0.0121 (9)
N1A	0.0455 (10)	0.0541 (11)	0.0483 (10)	-0.0116 (8)	0.0207 (8)	-0.0102 (8)
N2A	0.0446 (9)	0.0484 (10)	0.0447 (9)	-0.0100 (8)	0.0126 (7)	0.0000 (7)
C1A	0.0488 (12)	0.0684 (15)	0.0434 (11)	-0.0221 (11)	0.0171 (9)	-0.0073 (10)
C2A	0.0458 (11)	0.0622 (14)	0.0445 (11)	-0.0206(10)	0.0131 (9)	0.0012 (10)
C3A	0.0384 (10)	0.0422 (10)	0.0437 (10)	-0.0133(8)	0.0131 (8)	-0.0026(8)
C4A	0.0417 (10)	0.0447 (11)	0.0438 (10)	-0.0138(9)	0.0162 (8)	-0.0058(8)
C5A	0.0407 (11)	0.0494 (12)	0.0545(12)	-0.0074(9)	0.0178(9)	-0.0061(9)
C6A	0.0423(11)	0.0549(13)	0.0471(11)	-0.0126(10)	0 0095 (9)	-0.0019(9)
C7A	0.0468(11)	0.0556(13)	0.0430(10)	-0.0129(10)	0.0180 (9)	-0.0093(9)
C8A	0.0415(11)	0.0330(13) 0.0485(12)	0.0488(11)	-0.0077(9)	0.0100(9) 0.0173(8)	-0.0051(9)
C9A	0.0696 (16)	0.0543(12)	0.0594(13)	-0.0053(12)	0.0175(0)	-0.0142(11)
	0.0090(10)	0.0545(14) 0.0690(16)	0.0574(13) 0.0523(12)	0.0055(12)	0.0273(12) 0.0218(10)	-0.0142(11)
	0.0300(14) 0.0734(10)	0.0000(10)	0.0525(12) 0.0725(18)	0.0075(12)	0.0213(10)	0.0145(11)
CI1A C12A	0.0734(19)	0.125(5)	0.0723(18)	0.035(2)	0.0303(13) 0.0183(16)	-0.0050(13)
C12A	0.0002(13)	0.225(0)	0.074(2)	-0.002(2)	0.0183(10) 0.0270(16)	-0.021(3)
CIJA	0.0471(17)	0.203(3)	0.088(2)	-0.002(2)	0.0270(10)	-0.031(3)
CI4A	0.0555(10)	0.125(3)	0.092(2)	-0.0155(18)	0.0360(16)	-0.016(2)
CISA	0.0499 (13)	0.0809 (18)	0.0682 (15)	-0.0032(13)	0.0221 (11)	-0.0108(14)
CI6A	0.0571 (13)	0.0433 (12)	0.0575 (13)	-0.0031 (10)	0.0135 (10)	0.0036 (10)
CI/A	0.04/1 (12)	0.0470 (12)	0.0550 (12)	0.0051 (10)	0.0111 (9)	0.0001 (10)
C18A	0.0598 (15)	0.0776 (18)	0.0579 (14)	0.0104 (13)	0.0109 (11)	0.0062 (13)
C19A	0.0545 (16)	0.108 (3)	0.0772 (19)	0.0088 (17)	-0.0048 (14)	-0.0033 (18)
C20A	0.0480 (15)	0.087 (2)	0.115 (3)	-0.0072 (15)	0.0055 (16)	0.005 (2)
C21A	0.0598 (17)	0.090 (2)	0.107 (2)	-0.0122 (16)	0.0174 (16)	0.0273 (19)
C22A	0.0528 (14)	0.0783 (18)	0.0693 (16)	-0.0042 (13)	0.0051 (12)	0.0176 (14)
Cl1B	0.0706 (4)	0.0975 (6)	0.0804 (5)	0.0044 (4)	0.0372 (3)	-0.0286 (4)
O1B	0.0565 (9)	0.0892 (13)	0.0397 (8)	-0.0030 (9)	0.0152 (7)	-0.0119 (8)
O2B	0.0569 (9)	0.0730 (11)	0.0633 (10)	0.0107 (9)	0.0242 (8)	-0.0098 (9)
N1B	0.0373 (8)	0.0538 (10)	0.0380 (8)	-0.0033 (8)	0.0101 (6)	-0.0017 (7)
N2B	0.0373 (9)	0.0470 (10)	0.0455 (9)	-0.0039 (7)	0.0114 (7)	-0.0022 (7)
C1B	0.0376 (10)	0.0563 (12)	0.0423 (10)	-0.0089 (9)	0.0144 (8)	-0.0090 (9)
C2B	0.0400 (10)	0.0522 (12)	0.0480 (11)	-0.0046 (9)	0.0163 (8)	-0.0062 (9)
C3B	0.0399 (10)	0.0421 (10)	0.0408 (10)	-0.0103 (8)	0.0117 (8)	-0.0045 (8)
C4B	0.0376 (10)	0.0446 (11)	0.0404 (10)	-0.0103 (8)	0.0133 (8)	-0.0070 (8)
C5B	0.0419 (11)	0.0521 (12)	0.0477 (11)	-0.0036 (10)	0.0121 (9)	-0.0075 (9)
C6B	0.0568 (13)	0.0551 (13)	0.0544 (12)	-0.0127 (11)	0.0259 (10)	-0.0167 (10)
C7B	0.0641 (14)	0.0597 (14)	0.0402 (11)	-0.0143 (11)	0.0174 (10)	-0.0090 (10)
C8B	0.0537 (12)	0.0506 (12)	0.0413 (10)	-0.0104 (10)	0.0104 (9)	-0.0014 (9)
C9B	0.0514 (12)	0.0617 (14)	0.0475 (11)	0.0005 (11)	0.0136 (9)	0.0070 (10)
C10B	0.0468(12)	0.0740 (16)	0.0419 (11)	0.0031 (11)	0.0084 (9)	0.0051 (10)
C11B	0.0551(15)	0.081(2)	0.086(2)	-0.0020(14)	0.0062(14)	-0.0088(16)
C12B	0.066(2)	0.114(3)	0.098(2)	-0.027(2)	0.0002(17)	-0.002(2)
C13B	0.000(2) 0.0479(17)	0.161(4)	0.090(2) 0.087(2)	-0.012(2)	0.0020(17) 0.0027(14)	0.002(2)
C14B	0.0521(18)	0 145 (4)	0.115(3)	0.012(2)	0.0027(17)	0.020(3)
C15B	0.0609(17)	0.091(2)	0.096(2)	0.027(2) 0.0137(16)	0.0063(15)	0.020(3)
C16B	0.0452(11)	0.0469(12)	0.050(2)	-0.0024(9)	0.0128 (9)	0.0079(10)
C17R	0.0752(11) 0.0408(10)	0.0405(12)	0.0377(12)	0.002 + (7)	0.0120(9)	-0.0012(8)
\mathbf{U}	0.0400(10)	0.0770(11)	0.0727(10)	0.0037 (7)	0.0127(0)	0.0012 (0)

data reports

C18B	0.0523 (13)	0.0787 (17)	0.0517 (12)	0.0067 (12)	0.0113 (10)	0.0151 (12)
C19B	0.0472 (14)	0.110 (2)	0.0658 (16)	0.0030 (15)	-0.0046 (12)	0.0118 (16)
C20B	0.0448 (14)	0.089 (2)	0.092 (2)	-0.0110 (14)	0.0015 (13)	-0.0024 (17)
C21B	0.0602 (16)	0.0688 (18)	0.094 (2)	-0.0184 (14)	0.0098 (14)	0.0180 (15)
C22B	0.0526 (13)	0.0600 (14)	0.0611 (14)	-0.0087 (11)	-0.0009 (10)	0.0151 (12)

Geometric parameters (Å, °)

Cl1A—C6A	1.748 (2)	Cl1B—C6B	1.737 (2)
O1A—C1A	1.218 (3)	O1B—C1B	1.214 (3)
O2A—C2A	1.217 (3)	O2B—C2B	1.220 (3)
N1A—C1A	1.366 (3)	N1B—C1B	1.364 (3)
N1A—C4A	1.407 (3)	N1B—C4B	1.407 (2)
N1A—C9A	1.474 (3)	N1B—C9B	1.470 (3)
N2A—C2A	1.362 (3)	N2B—C2B	1.362 (3)
N2A—C3A	1.406 (3)	N2B—C3B	1.409 (3)
N2A—C16A	1.482 (3)	N2B—C16B	1.472 (3)
C1A—C2A	1.513 (4)	C1B—C2B	1.515 (3)
C3A—C4A	1.400 (3)	C3B—C4B	1.400 (3)
C3A—C8A	1.398 (3)	C3B—C8B	1.391 (3)
C4A—C5A	1.392 (3)	C4B—C5B	1.393 (3)
C5A—H5A	0.9300	C5B—H5B	0.9300
C5A—C6A	1.375 (3)	C5B—C6B	1.384 (3)
C6A—C7A	1.377 (3)	C6B—C7B	1.364 (4)
C7A—H7A	0.9300	C7B—H7B	0.9300
C7A—C8A	1.380 (3)	C7B—C8B	1.383 (3)
C8A—H8A	0.9300	C8B—H8B	0.9300
С9А—Н9АА	0.9700	С9В—Н9ВА	0.9700
С9А—Н9АВ	0.9700	C9B—H9BB	0.9700
C9A—C10A	1.502 (4)	C9B—C10B	1.514 (3)
C10A—C11A	1.383 (4)	C10B—C11B	1.365 (4)
C10A—C15A	1.379 (4)	C10B—C15B	1.379 (4)
C11A—H11A	0.9300	C11B—H11B	0.9300
C11A—C12A	1.401 (6)	C11B—C12B	1.392 (4)
C12A—H12A	0.9300	C12B—H12B	0.9300
C12A—C13A	1.363 (7)	C12B—C13B	1.351 (6)
C13A—H13A	0.9300	C13B—H13B	0.9300
C13A—C14A	1.363 (6)	C13B—C14B	1.356 (6)
C14A—H14A	0.9300	C14B—H14B	0.9300
C14A—C15A	1.376 (4)	C14B—C15B	1.385 (5)
C15A—H15A	0.9300	C15B—H15B	0.9300
C16A—H16A	0.9700	C16B—H16C	0.9700
C16A—H16B	0.9700	C16B—H16D	0.9700
C16A—C17A	1.508 (3)	C16B—C17B	1.504 (3)
C17A—C18A	1.390 (3)	C17B—C18B	1.387 (3)
C17A—C22A	1.378 (4)	C17B—C22B	1.376 (3)
C18A—H18A	0.9300	C18B—H18B	0.9300
C18A—C19A	1.390 (4)	C18B—C19B	1.374 (4)

C101 TT101		2105 X105	
C19A—H19A	0.9300	C19B—H19B	0.9300
C19A—C20A	1.359 (5)	C19B—C20B	1.365 (5)
C20A—H20A	0.9300	C20B—H20B	0.9300
C20A—C21A	1.374 (5)	C20B—C21B	1.369 (4)
C21A—H21A	0.9300	C21B—H21B	0.9300
C_{21} C_{22}	1.380(4)	C21B C22B	1.382(4)
C2IA—C22A	1.360 (4)		1.362 (4)
C22A—H22A	0.9300	C22B—H22B	0.9300
C1A—N1A—C4A	121.9 (2)	C1B—N1B—C4B	121.89 (18)
C1A—N1A—C9A	117.70 (19)	C1B—N1B—C9B	117.92 (18)
C4A—N1A—C9A	120.2 (2)	C4B—N1B—C9B	120.02 (18)
C2A—N2A—C3A	122.26 (19)	C2B—N2B—C3B	122.42 (18)
C2A—N2A—C16A	115.41 (19)	C2B—N2B—C16B	116.56 (18)
C3A - N2A - C16A	122 29 (18)	C3B - N2B - C16B	120.96 (17)
O1A $C1A$ $N1A$	122.29(10) 123.3(2)	OIB CIB NIB	123.0(2)
OIA - CIA - OIA	123.3(2)	OID - CID - OID	123.0(2)
UIA—CIA—C2A	118.9 (2)		119.2 (2)
NIA—CIA—C2A	117.75 (19)	NIB—CIB—C2B	117.83 (18)
O2A—C2A—N2A	122.7 (2)	O2B—C2B—N2B	122.8 (2)
O2A—C2A—C1A	119.0 (2)	O2B—C2B—C1B	119.1 (2)
N2A—C2A—C1A	118.3 (2)	N2B—C2B—C1B	118.04 (18)
C4A—C3A—N2A	119.30 (18)	C4B—C3B—N2B	118.95 (18)
C8A—C3A—N2A	121.74 (19)	C8B—C3B—N2B	121.8 (2)
C8A—C3A—C4A	118.96 (19)	C8B—C3B—C4B	119.2 (2)
$C_{3}A - C_{4}A - N_{1}A$	120.23(19)	C_{3B} C_{4B} N_{1B}	120.27(18)
$C_{5A} = C_{4A} = N_{1A}$	120.23(17)	C5D C4D N1D	120.27(10)
CSA—C4A—NIA	120.5(2)	C_{3B} C_{4B} C_{3B} C_{4B} C_{3B}	120.35 (19)
CSA—C4A—C3A	119.31 (19)	C5B—C4B—C3B	119.38 (19)
C4A—C5A—H5A	120.1	C4B—C5B—H5B	120.3
C6A—C5A—C4A	119.9 (2)	C6B—C5B—C4B	119.5 (2)
C6A—C5A—H5A	120.1	C6B—C5B—H5B	120.3
C5A—C6A—Cl1A	118.80 (18)	C5B—C6B—C11B	118.4 (2)
C5A—C6A—C7A	122.1 (2)	C7B—C6B—C11B	119.86 (18)
C7A—C6A—Cl1A	119.12 (17)	C7B—C6B—C5B	121.7 (2)
С6А—С7А—Н7А	120.9	C6B—C7B—H7B	120.5
C6A - C7A - C8A	1182(2)	C6B-C7B-C8B	1190(2)
C_{8A} C_{7A} H_{7A}	120.0	C8B C7B H7B	120.5
$C_{A} = C_{A} = H_{A}$	120.9	$C_{0}D_{-}C_{1}D_{-}H_{1}D_{-}$	120.5
C3A = C8A = H8A	119.2	$C3B - C\delta B - H\delta B$	119.5
C/A—C8A—C3A	121.6 (2)	C/B—C8B—C3B	121.0 (2)
С7А—С8А—Н8А	119.2	C7B—C8B—H8B	119.5
N1A—C9A—H9AA	109.0	N1B—C9B—H9BA	108.7
N1A—C9A—H9AB	109.0	N1B—C9B—H9BB	108.7
N1A-C9A-C10A	113.0 (2)	N1B-C9B-C10B	114.3 (2)
Н9АА—С9А—Н9АВ	107.8	Н9ВА—С9В—Н9ВВ	107.6
С10А—С9А—Н9АА	109.0	C10B—C9B—H9BA	108.7
С10А—С9А—Н9АВ	109.0	C10B—C9B—H9BB	108.7
C11A - C10A - C9A	120.7 (3)	C11B-C10B-C9B	122 5 (2)
C15A - C10A - C9A	120.7(3) 120.4(2)	C11B - C10B - C15B	1178(3)
C_{15} C_{10} C_{11} C_{11}	120.7(2) 1180(2)	C_{15} C_{10} C_{15} C_{15} C_{10} C	117.0(3)
CIDA CILA ULLA	110.9 (3)		119.7 (3)
UIUA—UITA—HITA	120.2		119.4

1197(4)	C10B—C11B—C12B	121 2 (3)
120.2	C12B—C11B—H11B	119.4
120.1	C11B—C12B—H12B	119.9
119.9 (4)	C13B—C12B—C11B	120.1 (4)
120.1	C13B—C12B—H12B	119.9
119.7	C12B—C13B—H13B	120.2
120.6 (3)	C12B—C13B—C14B	119.6 (3)
119.7	C14B—C13B—H13B	120.2
120.0	C13B—C14B—H14B	119.7
119.9 (4)	C13B—C14B—C15B	120.7 (4)
120.0	C15B—C14B—H14B	119.7
119.5	C10B—C15B—C14B	120.6 (4)
121.0 (3)	C10B—C15B—H15B	119.7
119.5	C14B—C15B—H15B	119.7
109.0	N2B—C16B—H16C	108.7
109.0	N2B—C16B—H16D	108.7
112.97 (18)	N2B-C16B-C17B	114.08 (18)
107.8	H16C—C16B—H16D	107.6
109.0	C17B—C16B—H16C	108.7
109.0	C17B—C16B—H16D	108.7
120.2 (2)	C18B—C17B—C16B	117.9 (2)
121.7 (2)	C22B—C17B—C16B	123.27 (19)
118.1 (2)	C22B—C17B—C18B	118.8 (2)
120.0	C17B—C18B—H18B	119.8
120.1 (3)	C19B—C18B—C17B	120.4 (3)
120.0	C19B—C18B—H18B	119.8
119.6	C18B—C19B—H19B	119.7
120.9 (3)	C20B—C19B—C18B	120.6 (3)
119.6	C20B—C19B—H19B	119.7
120.2	C19B—C20B—H20B	120.4
119.6 (3)	C19B—C20B—C21B	119.3 (3)
120.2	C21B—C20B—H20B	120.4
120.0	C20B—C21B—H21B	119.6
120.0 (3)	C20B—C21B—C22B	120.9 (3)
120.0	C22B—C21B—H21B	119.6
121.4 (3)	C17B—C22B—C21B	120.0 (2)
119.3	C17B—C22B—H22B	120.0
119.3	C21B—C22B—H22B	120.0
	119.7 (4) 120.2 120.1 $119.9 (4)$ 120.1 119.7 $120.6 (3)$ 119.7 120.0 $119.9 (4)$ 120.0 $119.9 (4)$ 120.0 119.5 $121.0 (3)$ 119.5 109.0 109.0 109.0 $112.97 (18)$ 107.8 109.0 109.0 $120.2 (2)$ $121.7 (2)$ $118.1 (2)$ 120.0 $120.1 (3)$ 120.0 119.6 120.2 $119.6 (3)$ 120.2 $120.0 (3)$ 120.0 $121.4 (3)$ 119.3	119.7 (4) $C10B-C11B-C12B$ 120.2 $C12B-C11B-H11B$ 120.1 $C11B-C12B-H12B$ 119.9 (4) $C13B-C12B-C11B$ 120.1 $C13B-C12B-H12B$ 119.7 $C12B-C13B-H13B$ 120.6 (3) $C12B-C13B-C14B$ 119.7 $C14B-C13B-H13B$ 120.0 $C13B-C14B-H14B$ 119.9 (4) $C13B-C14B-H14B$ 119.5 $C10B-C15B-C14B$ 120.0 $C15B-C14B-H14B$ 19.5 $C10B-C15B-C14B$ 19.5 $C10B-C15B-H15B$ 19.5 $C14B-H16D$ 19.9 (4) $C13B-C16B-H16C$ 19.0 $N2B-C16B-H16D$ 19.5 $C14B-C16B-H16D$ 109.0 $N2B-C16B-H16D$ 112.97 (18) $N2B-C16B-H16D$ 109.0 $C17B-C16B-H16D$ 109.0 $C17B-C16B-H16D$ 120.2 (2) $C18B-C17B-C16B$ 118.1 (2) $C22B-C17B-C16B$ 120.0 $C19B-C18B-H18B$ 120.0 $C19B-C18B-H18B$ 120.1 (3) $C19B-C18B-H18B$ 120.9 (3) $C20B-C19B-H19B$ 120.2 $C1B-C20B-H20B$ 19.6 (3) $C19B-C20B-H20B$ 19.6 (3) $C19B-C20B-H20B$ 19.6 (3) $C20B-C21B-H21B$ 120.0 $C22B-C21B-H21B$ 120.0 $C20B-C21B-H22B$ 120.1 $C17B-C22B-C21B$ 120.2 $C21B-C22B-C21B$ 120.3 $C17B-C22B-C21B$ 120.4 (3) $C17B-C22B-C21B$ 120.5 $C21B-C22B-C21B$ 120.6 $C20B-C21B-H22B$

Hydrogen-bond geometry (Å, °)

D—H···A	<i>D</i> —Н	H···A	D···A	D—H···A
$C7A$ — $H7A$ ···O2 B^{i}	0.93	2.48	3.323 (3)	151
$C22A$ — $H22A$ ···O1 B^{i}	0.93	2.60	3.454 (3)	154
C7 <i>B</i> —H7 <i>B</i> ···O2 <i>A</i>	0.93	2.43	3.151 (3)	135
C18 <i>B</i> —H18 <i>B</i> …O1 <i>A</i>	0.93	2.72	3.353 (3)	126

Symmetry code: (i) x, -y+1/2, z+1/2.