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

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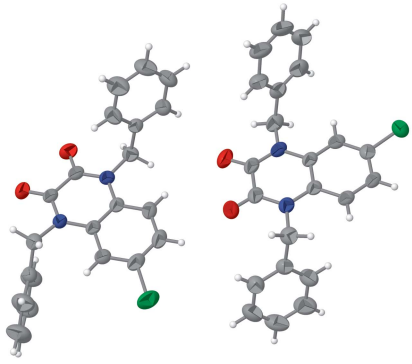
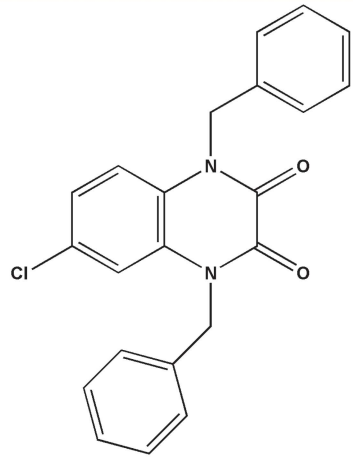
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $C_{22}H_{17}ClN_2O_2$, 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···O hydrogen bonds and π–π stacking interactions link the molecules into a three-dimensional network.

3D view



Chemical scheme



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(1*H*,4*H*)-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(1*H*,4*H*)-dione unit is essentially planar. The maximum r.m.s. deviation from the mean plane through the non-H atoms of ring *A* (N1*A*/C1*A*/C2*A*/N2*A*/C3*A*/C8*A*/C7*A*/C5*A*/C4*A*) is 0.053 (2) Å for N2*A* and for ring *B* (N1*B*/C1*B*/C2*B*/N2*B*/C3*B*/C8*B*/C7*B*/C5*B*/C4*B*) is 0.096 (2) Å for N2*B*. The dihedral angles between the mean plane of the 6-chloroquinoxaline-2,3(1*H*,4*H*)-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

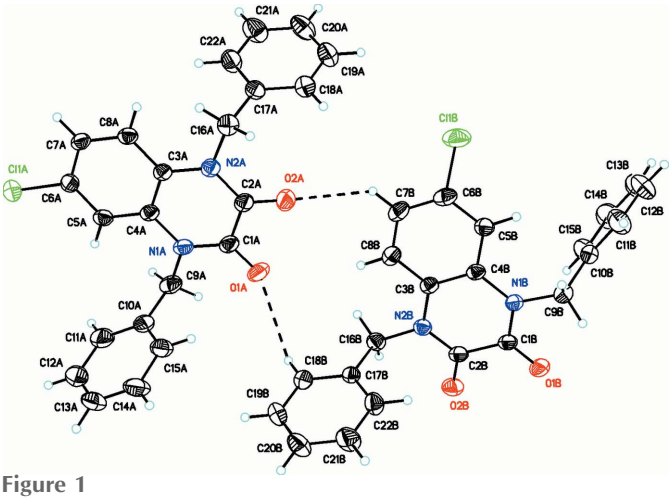


Figure 1
The molecular structure of the title compound, showing the atom-numbering scheme for molecules *A* and *B*, and 30% probability displacement ellipsoids for the non-H atoms. Dashed lines indicate weak C7*B*—H7*B*···O2*A* and C18*B*—H18*B*···O1*A* intermolecular interactions within the asymmetric 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 C7*B*—H7*B*···O2*A* and C18*B*—H18*B*···O1*A* interactions (Table 1) within the asymmetric unit (Fig. 1). Additional C—H···O hydrogen bonds, together with π–π stacking interactions [*Cg*2–*Cg*7^{ii} = 3.6611 (14) Å; symmetry code: (ii) $x, 1+y, z$; *Cg*2 and *Cg*7 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(1*H*,4*H*)-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 chromatographed 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.

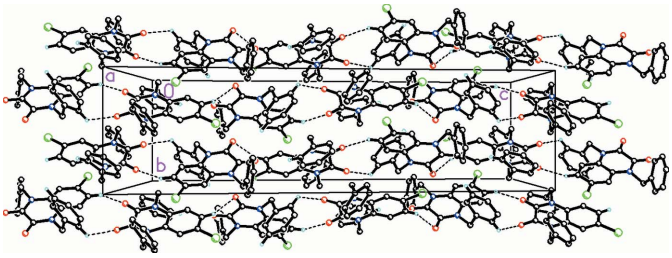


Figure 2
The packing of the title compound, viewed along the *a* axis. Dashed lines indicate intermolecular C—H···O interactions. H atoms not involved in the packing have been omitted for clarity.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7*A*—H7*A*···O2*B*^{i}	0.93	2.48	3.323 (3)	151
C22*A*—H22*A*···O1*B*^{i}	0.93	2.60	3.454 (3)	154
C7*B*—H7*B*···O2*A*	0.93	2.43	3.151 (3)	135
C18*B*—H18*B*···O1*A*	0.93	2.72	3.353 (3)	126

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{22}H_{17}ClN_2O_2$
M_r	376.82
Crystal system, space group	Monoclinic, *I*2/*a*
Temperature (K)	293
a, *b*, *c* (Å)	29.2234 (4), 8.3076 (2), 31.0407 (5)
β (°)	101.859 (2)
V (Å^3)	7375.1 (2)
Z	16
Radiation type	Cu *K*α
μ (mm^{-1})	1.99
Crystal size (mm)	0.28 × 0.24 × 0.12
Data collection	
Diffractometer	Rigaku Oxford Diffraction
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku Oxford Diffraction, 2015)
T_{min}, T_{max}	0.500, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	14412, 6996, 5661
R_{int}	0.022
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.614
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.053, 0.156, 1.04
No. of reflections	6996
No. of parameters	487
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.73, −0.37

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

Refinement

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

Acknowledgements

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full crystallographic data

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

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

Crystal data

$C_{22}H_{17}ClN_2O_2$
M_r = 376.82
Monoclinic, *I*2/*a*
a = 29.2234 (4) Å
b = 8.3076 (2) Å
c = 31.0407 (5) Å
β = 101.859 (2)°
V = 7375.1 (2) Å^3
Z = 16
F(000) = 3136
D_x = 1.358 Mg m^{-3}
Cu *Kα* radiation, *λ* = 1.54184 Å
Cell parameters from 6649 reflections
θ = 4.6–71.4°
μ = 1.99 mm^{-1}
T = 293 K
Prism, orange
0.28 × 0.24 × 0.12 mm

Data collection

Rigaku Oxford Diffraction diffractometer
Radiation source: fine-focus sealed X-ray tube, Enhance (Cu) X-ray Source
Graphite monochromator
Detector resolution: 16.0416 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlis PRO; Rigaku Oxford Diffraction, 2015)
T_{min} = 0.500, T_{max} = 1.000
14412 measured reflections
6996 independent reflections
5661 reflections with $I > 2\sigma(I)$
R_{int} = 0.022
θ_{max} = 71.3°, θ_{min} = 3.8°
h = −35→25
k = −10→9
l = −37→38

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.156
S = 1.04
6996 reflections
487 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0814P)^2 + 5.5513P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.73 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1A	0.62007 (2)	0.06298 (9)	0.71293 (2)	0.0677 (2)
O1A	0.53226 (7)	0.1255 (3)	0.47249 (6)	0.0740 (6)
O2A	0.46801 (6)	0.3455 (3)	0.48365 (6)	0.0655 (5)
N1A	0.55925 (6)	0.1082 (2)	0.54650 (6)	0.0477 (4)
N2A	0.48818 (6)	0.3198 (2)	0.55775 (6)	0.0454 (4)
C1A	0.53004 (8)	0.1662 (3)	0.50969 (7)	0.0524 (6)
C2A	0.49289 (8)	0.2857 (3)	0.51596 (7)	0.0503 (5)
C3A	0.51820 (7)	0.2548 (2)	0.59492 (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)	0.66737 (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)	0.0451 (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	0.67930 (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	0.37076 (10)	0.3851 (4)	0.51459 (9)	0.0653 (7)
H18A	0.3790	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	0.2840	0.1773	0.5347	0.102*
C21A	0.34496 (11)	0.1960 (4)	0.57839 (13)	0.0856 (10)
H21A	0.3363	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*
Cl1B	0.33081 (3)	0.58144 (10)	0.37621 (3)	0.0797 (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 (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1A	0.0533 (3)	0.0909 (5)	0.0550 (3)	−0.0014 (3)	0.0025 (2)	0.0022 (3)

O1A	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)	0.0485 (12)	0.0488 (11)	−0.0077 (9)	0.0173 (8)	−0.0051 (9)
C9A	0.0696 (16)	0.0543 (14)	0.0594 (13)	−0.0053 (12)	0.0275 (12)	−0.0142 (11)
C10A	0.0566 (14)	0.0690 (16)	0.0523 (12)	0.0075 (12)	0.0218 (10)	−0.0145 (11)
C11A	0.0734 (19)	0.125 (3)	0.0725 (18)	0.035 (2)	0.0303 (15)	0.0056 (19)
C12A	0.0602 (19)	0.225 (6)	0.074 (2)	0.046 (3)	0.0183 (16)	−0.006 (3)
C13A	0.0471 (17)	0.205 (5)	0.088 (2)	−0.002 (2)	0.0270 (16)	−0.031 (3)
C14A	0.0553 (16)	0.125 (3)	0.092 (2)	−0.0153 (18)	0.0360 (16)	−0.016 (2)
C15A	0.0499 (13)	0.0809 (18)	0.0682 (15)	−0.0032 (13)	0.0221 (11)	−0.0108 (14)
C16A	0.0571 (13)	0.0433 (12)	0.0575 (13)	−0.0031 (10)	0.0135 (10)	0.0036 (10)
C17A	0.0471 (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)	0.0026 (17)	−0.002 (2)
C13B	0.0479 (17)	0.161 (4)	0.087 (2)	−0.012 (2)	0.0027 (14)	0.019 (3)
C14B	0.0521 (18)	0.145 (4)	0.115 (3)	0.027 (2)	0.0084 (17)	0.020 (3)
C15B	0.0609 (17)	0.091 (2)	0.096 (2)	0.0137 (16)	0.0063 (15)	0.0105 (18)
C16B	0.0452 (11)	0.0469 (12)	0.0549 (12)	−0.0024 (9)	0.0128 (9)	0.0079 (10)
C17B	0.0408 (10)	0.0445 (11)	0.0427 (10)	0.0037 (9)	0.0124 (8)	−0.0012 (8)

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, º)

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
C9A—H9AA	0.9700	C9B—H9BA	0.9700
C9A—H9AB	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)

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
C21A—C22A	1.380 (4)	C21B—C22B	1.382 (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	123.3 (2)	O1B—C1B—N1B	123.0 (2)
O1A—C1A—C2A	118.9 (2)	O1B—C1B—C2B	119.2 (2)
N1A—C1A—C2A	117.75 (19)	N1B—C1B—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)
C3A—C4A—N1A	120.23 (19)	C3B—C4B—N1B	120.27 (18)
C5A—C4A—N1A	120.5 (2)	C5B—C4B—N1B	120.35 (19)
C5A—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—Cl1B	118.4 (2)
C5A—C6A—C7A	122.1 (2)	C7B—C6B—Cl1B	119.86 (18)
C7A—C6A—Cl1A	119.12 (17)	C7B—C6B—C5B	121.7 (2)
C6A—C7A—H7A	120.9	C6B—C7B—H7B	120.5
C6A—C7A—C8A	118.2 (2)	C6B—C7B—C8B	119.0 (2)
C8A—C7A—H7A	120.9	C8B—C7B—H7B	120.5
C3A—C8A—H8A	119.2	C3B—C8B—H8B	119.5
C7A—C8A—C3A	121.6 (2)	C7B—C8B—C3B	121.0 (2)
C7A—C8A—H8A	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)
H9AA—C9A—H9AB	107.8	H9BA—C9B—H9BB	107.6
C10A—C9A—H9AA	109.0	C10B—C9B—H9BA	108.7
C10A—C9A—H9AB	109.0	C10B—C9B—H9BB	108.7
C11A—C10A—C9A	120.7 (3)	C11B—C10B—C9B	122.5 (2)
C15A—C10A—C9A	120.4 (2)	C11B—C10B—C15B	117.8 (3)
C15A—C10A—C11A	118.9 (3)	C15B—C10B—C9B	119.7 (3)
C10A—C11A—H11A	120.2	C10B—C11B—H11B	119.4

C10A—C11A—C12A	119.7 (4)	C10B—C11B—C12B	121.2 (3)
C12A—C11A—H11A	120.2	C12B—C11B—H11B	119.4
C11A—C12A—H12A	120.1	C11B—C12B—H12B	119.9
C13A—C12A—C11A	119.9 (4)	C13B—C12B—C11B	120.1 (4)
C13A—C12A—H12A	120.1	C13B—C12B—H12B	119.9
C12A—C13A—H13A	119.7	C12B—C13B—H13B	120.2
C12A—C13A—C14A	120.6 (3)	C12B—C13B—C14B	119.6 (3)
C14A—C13A—H13A	119.7	C14B—C13B—H13B	120.2
C13A—C14A—H14A	120.0	C13B—C14B—H14B	119.7
C13A—C14A—C15A	119.9 (4)	C13B—C14B—C15B	120.7 (4)
C15A—C14A—H14A	120.0	C15B—C14B—H14B	119.7
C10A—C15A—H15A	119.5	C10B—C15B—C14B	120.6 (4)
C14A—C15A—C10A	121.0 (3)	C10B—C15B—H15B	119.7
C14A—C15A—H15A	119.5	C14B—C15B—H15B	119.7
N2A—C16A—H16A	109.0	N2B—C16B—H16C	108.7
N2A—C16A—H16B	109.0	N2B—C16B—H16D	108.7
N2A—C16A—C17A	112.97 (18)	N2B—C16B—C17B	114.08 (18)
H16A—C16A—H16B	107.8	H16C—C16B—H16D	107.6
C17A—C16A—H16A	109.0	C17B—C16B—H16C	108.7
C17A—C16A—H16B	109.0	C17B—C16B—H16D	108.7
C18A—C17A—C16A	120.2 (2)	C18B—C17B—C16B	117.9 (2)
C22A—C17A—C16A	121.7 (2)	C22B—C17B—C16B	123.27 (19)
C22A—C17A—C18A	118.1 (2)	C22B—C17B—C18B	118.8 (2)
C17A—C18A—H18A	120.0	C17B—C18B—H18B	119.8
C17A—C18A—C19A	120.1 (3)	C19B—C18B—C17B	120.4 (3)
C19A—C18A—H18A	120.0	C19B—C18B—H18B	119.8
C18A—C19A—H19A	119.6	C18B—C19B—H19B	119.7
C20A—C19A—C18A	120.9 (3)	C20B—C19B—C18B	120.6 (3)
C20A—C19A—H19A	119.6	C20B—C19B—H19B	119.7
C19A—C20A—H20A	120.2	C19B—C20B—H20B	120.4
C19A—C20A—C21A	119.6 (3)	C19B—C20B—C21B	119.3 (3)
C21A—C20A—H20A	120.2	C21B—C20B—H20B	120.4
C20A—C21A—H21A	120.0	C20B—C21B—H21B	119.6
C20A—C21A—C22A	120.0 (3)	C20B—C21B—C22B	120.9 (3)
C22A—C21A—H21A	120.0	C22B—C21B—H21B	119.6
C17A—C22A—C21A	121.4 (3)	C17B—C22B—C21B	120.0 (2)
C17A—C22A—H22A	119.3	C17B—C22B—H22B	120.0
C21A—C22A—H22A	119.3	C21B—C22B—H22B	120.0

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7*A*—H7*A*···O2*B*^{i}	0.93	2.48	3.323 (3)	151
C22*A*—H22*A*···O1*B*^{i}	0.93	2.60	3.454 (3)	154
C7*B*—H7*B*···O2*A*	0.93	2.43	3.151 (3)	135
C18*B*—H18*B*···O1*A*	0.93	2.72	3.353 (3)	126

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