organic compounds

7,9-Dichloro-6*H*,12*H*-indolo[2,1-*b*]-quinazoline-6,12-dione

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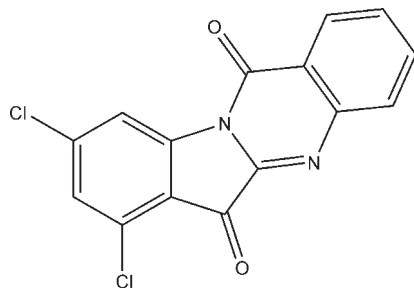Correspondence e-mail: pgrundt@d.umn.edu, vnemykin@d.umn.edu

There are two independent molecules in the asymmetric unit of the title compound, $C_{15}H_6Cl_2N_2O_2$. The conjugated four-ring system is essentially planar in each molecule [maximum deviation = 0.089 (2) Å]. In the crystal, weak intermolecular C—H⋯Cl, C—H⋯O and C—H⋯N interactions help to stabilize the packing.

Related literature

For the synthesis, chemistry, and biological activity of the title compound see: Krivogorsky *et al.* (2008). For chemistry and biological activity of the natural product tryptanthrin (indolo[2,1-*b*]quinazoline-6,12-dione) and its derivatives and for related structures, see: Honda *et al.* (1979); Mitscher & Baker (1998); Kataoka *et al.* (2001); Bandekar *et al.* (2010); Sharma *et al.* (2002); Motoki *et al.* (2005); Yu *et al.* (2009); Bhattacharjee *et al.* (2002); Scovill *et al.* (2002); Bhattacharjee *et al.* (2004); Pitzer *et al.* (2000). For the extinction correction, see: Larson (1970).

Experimental

Crystal data

$C_{15}H_6Cl_2N_2O_2$	b = 10.7276 (3) Å
M_r = 317.13	c = 17.2338 (12) Å
Triclinic, $P\bar{1}$	α = 94.908 (7)°
a = 7.0179 (2) Å	β = 96.709 (7)°

γ = 107.395 (8)°	μ = 0.54 mm^{-1}
V = 1219.66 (12) Å^3	T = 100 K
Z = 4	0.54 × 0.48 × 0.35 mm
Mo $K\alpha$ radiation	

Data collection

Rigaku R-AXIS RAPID-II imaging plate diffractometer	31502 measured reflections
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)	5585 independent reflections
T_{min} = 0.633, T_{max} = 0.899	4830 reflections with $I > 2\sigma(I)$
	R_{int} = 0.049

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034	84 restraints
$wR(F^2)$ = 0.082	All H-atom parameters refined
S = 1.00	$\Delta\rho_{max}$ = 0.53 e Å^{-3}
5571 reflections	$\Delta\rho_{min}$ = −0.36 e Å^{-3}
416 parameters	

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
C1B—H1B⋯Cl1A^i	0.94 (2)	2.73 (2)	3.637 (2)	162 (1)
C2A—H2A⋯O1B^{ii}	0.93 (2)	2.54 (2)	3.264 (3)	135 (1)
C4B—H4B⋯N5A^{iii}	0.94 (2)	2.56 (2)	3.422 (3)	154 (1)
C10A—H6A⋯Cl2B^{iv}	0.94 (2)	2.67 (2)	3.585 (2)	165 (1)

Symmetry codes: (i) $-x, -y + 1, -z$; (ii) $-x + 2, -y, -z$; (iii) $x - 1, y, z$; (iv) $x, y - 1, z - 1$.

Data collection: *CrystalClear* (Rigaku Americas, 2009); cell refinement: *HKL-2000* (Otwinowski & Minor, 1997); data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS86* (Sheldrick, 2008); program(s) used to refine structure: *CRYSTALS* (Betteridge *et al.*, 2003); molecular graphics: *CAMERON* (Watkin *et al.*, 1996); software used to prepare material for publication: *CRYSTALS*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: JJ2032).

References

Bandekar, P. P., Roopnarine, K. A., Parekh, V. J., Mitchell, T. R., Novak, M. J. & Sinden, R. R. (2010). *J. Med. Chem.* **53**, 3558–3565.
Betteridge, P. W., Carruthers, J. R., Cooper, R. I., Prout, K. & Watkin, D. J. (2003). *J. Appl. Cryst.* **36**, 1487.
Bhattacharjee, A. K., Hartell, M. G., Nichols, D. A., Hicks, R. P., Stanton, B., Van Hamont, J. E. & Milhous, W. K. (2004). *Eur. J. Med. Chem.* **39**, 59–67.
Bhattacharjee, A. K., Skanchy, D. J., Jennings, B., Hudson, T. H., Brendle, J. J. & Werbovetz, K. A. (2002). *Bioorg. Med. Chem.* **10**, 1979–1989.
Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
Honda, G., Tabata, M. & Tsuda, M. (1979). *Planta Med.* **37**, 172–174.
Kataoka, M., Hirata, K., Kunikata, T., Ushio, S., Iwaki, K., Ohashi, K., Ikeda, M. & Kurimoto, M. (2001). *J. Gastroenterol.* **36**, 5–9.
Krivogorsky, B., Grundt, P., Yolken, R. & Jones-Brando, L. (2008). *Antimicrob. Agents Chemother.* **52**, 4466–4469.
Larson, A. C. (1970). *Crystallographic Computing*, edited by F. R. Ahmed, S. R. Hall & C. P. Huber, pp. 291–294. Copenhagen: Munksgaard.
Mitscher, L. A. & Baker, W. R. (1998). *Pure Appl. Chem.* **70**, 365–371.
Motoki, T., Takami, Y., Yagi, Y., Tai, A., Yamamoto, I. & Gohda, E. (2005). *Biol. Pharm. Bull.* **28**, 260–266.

Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr & R. M. Sweet, pp. 307–326. New York: Academic Press.

Pitzer, K. K., Scovill, J. P, Kyle, D. E. & Gerena, L. (2000). [WRAIR (Walter Reid Army Institute of Research), USA]. 99-US22569 2000018769.

Rigaku Americas (2009). *CrystalStructure*. Rigaku Americas, The Woodlands, Texas, USA.

Scovill, J., Blank, E., Konnick, M., Nenortas, E. & Shapiro, T. (2002). *Antimicrob. Agents Chemother.* **46**, 882–883.

Sharma, V. M., Prasanna, P., Adi Seshu, K. V., Renuka, B., Laxman Rao, C. V., Sunil Kumar, G., Narasimhulu, C. P., Aravind Babu, P., Puranik, R. C., Subramanyam, D., Venkateswarlu, A., Rajagopal, S., Kumar, K. B. S., Rao, C. S., Mamidi, N. V. S. R., Deevi, D. S., Ajaykumar, R. & Rajagopalan, R. (2002). *Bioorg. Med. Chem. Lett.* **12**, 2303–2307.

Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

Watkin, D. J., Prout, C. K. & Pearce, L. J. (1996). *CAMERON*. Chemical Crystallography Laboratory, Oxford, England.

Yu, S.-T., Chen, T.-M., Chern, J.-W., Tseng, S.-Y. & Chen, Y.-H. (2009). *Anti-Cancer Drugs*, **20**, 382–388.

supporting information

7,9-Dichloro-6*H*,12*H*-indolo[2,1-*b*]quinazoline-6,12-dione

Peter Grundt, Kelsi A. Douglas, Bogdana Krivogorsky and Victor N. Nemykin

S1. Comment

The natural product tryptanthrin (indolo[2,1-b]quinazoline-6,12-dione) and its derivatives have been shown to possess antibacterial (Honda *et al.*, 1979), Mitscher & Baker, 1998, Kataoka *et al.*, 2001, Bandekar *et al.*, 2010) and antitumor Sharma *et al.*, 2002, Motoki *et al.*, 2005, Yu *et al.*, 2009) properties. Of particular interest is the discovery by several groups that this class of compounds also inibits the growth of parasites such as *Leishmania donovani* (Bhattacharjee *et al.*, 2002), *Trypanosoma brucei* (Scovill *et al.*, 2002), and *Plasmodium falciparum* (Bhattacharjee *et al.*, 2004, Pitzer *et al.*, 2000), and more recently by our laboratory, *Toxoplasma gondii* (Krivogorsky *et al.*, 2008). In our continued interest to characterize the structure-activity-relationship of this class of compounds and to reveal the underlying mechanism, we have synthesized the 7,9-dichloro analog of tryptanthrin.

The title compound, (I), $C_{15}H_6Cl_2N_2O_2$, crystallizes in the P-1 space group with two independent molecules in the asymmetric unit cell. It consists of a 7,9-dichloroindolo ring fused to a quinazoline ring with a dione group at the 6 and 12 poisitions (IUPAC nomenclature). C—Cl bond distances have been observed between 1.7272 (19) and 1.7358 (19) Å with Cl1—C7 distances being slightly shorter as compared to Cl2—C9 bond lengths. C=O bonds have clear double bond character and were observed between 1.211 (2) and 1.221 (2) Å with C=O bonds in the five-membered ring being slightly shorter as compared to those at the six-membered rings. N5—C14 bond distances in molecules A and B have clear double bond character. Four weak intermolecular interactions are observed in (I), (Table 2) that help stabilize crystal packing.

S2. Experimental

The title compound was prepared by condensation of isatoic anhydride and 4,6-dichloroisatin in refluxing benzene with triethylamine as a co-solvent (Krivogorsky *et al.*, 2008). Crystals suitable for single-crystal X-ray diffraction were grown by slow evaporation of an acetone solution of the compound.

S3. Refinement

In the absence of significant anomalous scattering, Friedel pairs were merged. The H atoms were all located in a difference map, but were repositioned geometrically. The H atoms were initially refined with soft restraints on the bond lengths and angles to regularize their geometry (C—H in the range 0.93–0.94 Å) and U_{iso}(H) (in the range 1.2–1.5 times U_{eq} of the parent atom), after which the positions were refined with riding constraints.
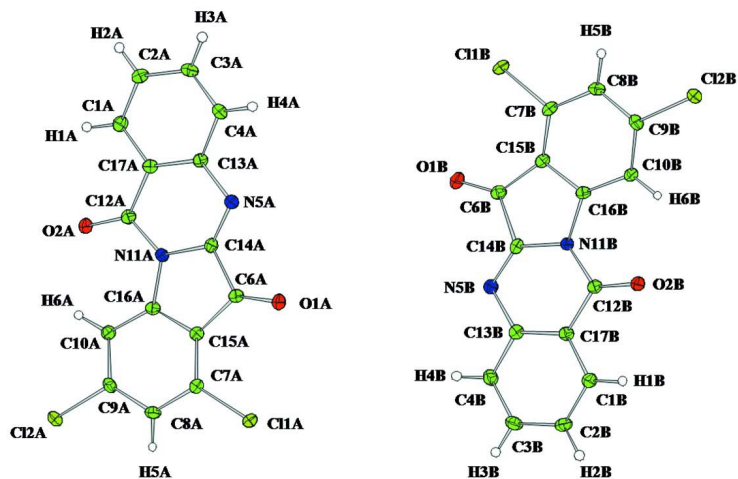
Figure 1

The title compound with displacement ellipsoids drawn at the 50% probability level. H atoms are shown as spheres of arbitary radius.
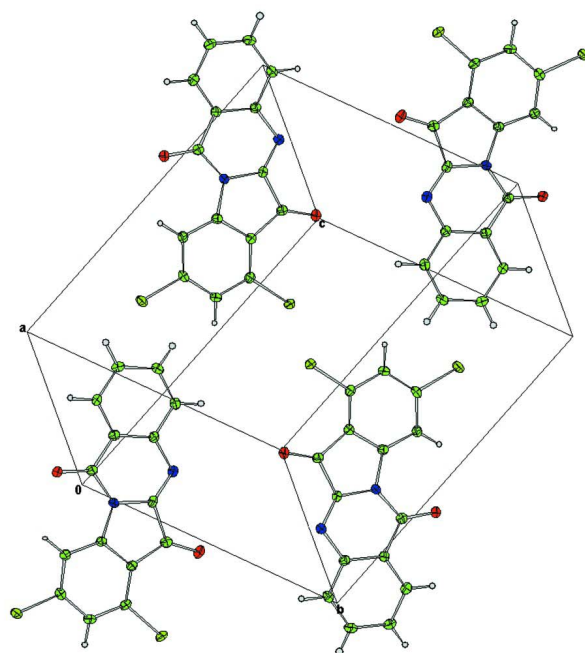
Figure 2

Packing diagram for the title compound with displacement ellipsoids drawn at the 50% probability level. H atoms are omited for clarity.

7,9-Dichloro-6H,12H-indolo[2,1-b]quinazoline-6,12-dione

Crystal data

$C_{15}H_6Cl_2N_2O_2$	$Z = 4$
$M_r = 317.13$	$F(000) = 640$
Triclinic, $P\overline{1}$	$D_x = 1.727$ Mg m^{-3}
Hall symbol: -P 1	Melting point: 200 K
$a = 7.0179$ (2) Å	Mo $K\alpha$ radiation, $\lambda = 0.71075$ Å
$b = 10.7276$ (3) Å	Cell parameters from 28356 reflections
$c = 17.2338$ (12) Å	$\theta = 3.1–27.5°$
$\alpha = 94.908$ (7)°	$\mu = 0.54$ mm^{-1}
$\beta = 96.709$ (7)°	$T = 100$ K
$\gamma = 107.395$ (8)°	Block, yellow
$V = 1219.66$ (12) Å^3	$0.54 \times 0.48 \times 0.35$ mm

Data collection

Rigaku R-AXIS RAPID-II imaging plate diffractometer	31502 measured reflections
	5585 independent reflections
Radiation source: Sealed tube (Mo)	4830 reflections with $I > 2\sigma(I)$
Graphite monochromator	$R_{int} = 0.049$
Detector resolution: 10 pixels mm^{-1}	$\theta_{max} = 27.5°$, $\theta_{min} = 3.1°$
ω scans	$h = -9\rightarrow9$
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	$k = -13\rightarrow13$
	$l = -22\rightarrow22$
$T_{min} = 0.633$, $T_{max} = 0.899$	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.034$	All H-atom parameters refined
$wR(F^2) = 0.082$	Method = Modified Sheldrick $w = 1/[\sigma^2(F^2) + (0.02P)^2 + 2.09P]$,
$S = 1.00$	where $P = [\max(F_o^2, 0) + 2F_c^2]/3$
5571 reflections	$(\Delta/\sigma)_{max} = 0.001$
416 parameters	$\Delta\rho_{max} = 0.53$ e Å^{-3}
84 restraints	$\Delta\rho_{min} = -0.36$ e Å^{-3}
0 constraints	Extinction correction: Larson (1970), Equation 22
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 43 (4)
Secondary atom site location: difference Fourier map	

Special details

Experimental. The crystal was placed in the cold stream of an X-stream 2000 liquid nitrogen generator with open-flow nitrogen cryostat with a nominal stability of 0.1 K. ^{1}H NMR (DMSO-d6, 500 MHz): d 7.75-7.78 (m, 2H), 7.98-8.00 (m, 2H), 8.33 (d, J 7.5, 1H), 8.41 (d, J 1.9, 1H). ^{13}C NMR (DMSO-d6, 125 MHz): d 115.6, 118.3, 122.6, 127.0, 127.4, 129.9, 130.1, 132.3, 135.6, 141.6, 144.4, 146.1, 147.3, 157.6, 178.4.

Refinement. Crystals for Windows program eliminates all reflections with [Sin theta/lambda]**2 less than 0.01 in order to eliminate reflections that may be poorly measured in the vicinity of the beam stop. Such filter eliminated 14 reflections, which resulted in difference between 5585 measured unique reflections and 5571 reflections used for refinement.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1A	0.12767 (7)	0.19849 (5)	−0.30745 (3)	0.0154
Cl2A	0.22470 (8)	−0.16786 (5)	−0.51632 (3)	0.0203
O1A	0.5092 (2)	0.25603 (14)	−0.16905 (8)	0.0172
O2A	0.8111 (2)	−0.15104 (14)	−0.30107 (8)	0.0181
C1A	1.1319 (3)	−0.08669 (19)	−0.17069 (12)	0.0162
C2A	1.2819 (3)	−0.0485 (2)	−0.10617 (12)	0.0183
C3A	1.2850 (3)	0.0523 (2)	−0.04843 (12)	0.0208
C4A	1.1391 (3)	0.1145 (2)	−0.05462 (12)	0.0185
N5A	0.8403 (2)	0.14280 (16)	−0.12490 (10)	0.0151
C6A	0.5402 (3)	0.16629 (19)	−0.20790 (11)	0.0137
C7A	0.2640 (3)	0.09548 (18)	−0.33341 (11)	0.0137
C8A	0.1974 (3)	0.01396 (19)	−0.40464 (11)	0.0154
C9A	0.3055 (3)	−0.06961 (19)	−0.42595 (11)	0.0151
C10A	0.4729 (3)	−0.07980 (19)	−0.37831 (11)	0.0146
N11A	0.6952 (2)	0.01079 (16)	−0.24828 (9)	0.0130
C12A	0.8273 (3)	−0.06404 (19)	−0.24787 (11)	0.0140
C13A	0.9855 (3)	0.07665 (19)	−0.11960 (11)	0.0142
C14A	0.7090 (3)	0.10816 (18)	−0.18691 (11)	0.0134
C15A	0.4331 (3)	0.09159 (18)	−0.28464 (11)	0.0129
C16A	0.5321 (3)	0.00196 (19)	−0.30772 (11)	0.0141
C17A	0.9828 (3)	−0.02472 (18)	−0.17809 (11)	0.0139
Cl1B	0.89170 (7)	0.34858 (5)	0.34019 (3)	0.0173
Cl2B	0.70190 (7)	0.70635 (5)	0.52404 (3)	0.0192

O1B	0.5337 (2)	0.26130 (14)	0.19080 (9)	0.0189
O2B	0.1512 (2)	0.64871 (14)	0.28391 (8)	0.0169
C1B	−0.1458 (3)	0.55847 (19)	0.14382 (12)	0.0163
C2B	−0.2819 (3)	0.5080 (2)	0.07583 (12)	0.0193
C3B	−0.2635 (3)	0.4038 (2)	0.02547 (12)	0.0192
C4B	−0.1086 (3)	0.3521 (2)	0.04302 (12)	0.0176
N5B	0.1872 (3)	0.34718 (16)	0.12667 (10)	0.0153
C6B	0.4831 (3)	0.34864 (19)	0.22288 (11)	0.0148
C7B	0.7333 (3)	0.44170 (19)	0.35489 (12)	0.0146
C8B	0.7737 (3)	0.5271 (2)	0.42418 (12)	0.0165
C9B	0.6463 (3)	0.60188 (19)	0.43630 (11)	0.0151
C10B	0.4808 (3)	0.59806 (19)	0.38219 (11)	0.0144
N11B	0.2930 (2)	0.49043 (16)	0.24801 (9)	0.0130
C12B	0.1523 (3)	0.55777 (19)	0.23644 (11)	0.0138
C13B	0.0312 (3)	0.40238 (18)	0.11173 (11)	0.0139
C14B	0.3049 (3)	0.39217 (19)	0.19191 (11)	0.0140
C15B	0.5689 (3)	0.43274 (19)	0.29911 (11)	0.0139
C16B	0.4478 (3)	0.51304 (19)	0.31342 (11)	0.0135
C17B	0.0111 (3)	0.50602 (19)	0.16292 (11)	0.0141
H1A	1.130 (2)	−0.1539 (13)	−0.2094 (9)	0.0204*
H2A	1.380 (2)	−0.0909 (13)	−0.1021 (9)	0.0206*
H3A	1.388 (2)	0.0793 (14)	−0.0051 (9)	0.0251*
H4A	1.142 (2)	0.1815 (13)	−0.0153 (9)	0.0215*
H5A	0.083 (2)	0.0145 (13)	−0.4368 (9)	0.0178*
H6A	0.541 (2)	−0.1385 (13)	−0.3938 (9)	0.0187*
H1B	−0.159 (2)	0.6286 (13)	0.1773 (9)	0.0204*
H2B	−0.388 (2)	0.5439 (14)	0.0634 (9)	0.0248*
H3B	−0.355 (2)	0.3688 (14)	−0.0209 (9)	0.0224*
H4B	−0.094 (2)	0.2847 (13)	0.0083 (9)	0.0208*
H5B	0.885 (2)	0.5353 (13)	0.4615 (9)	0.0195*
H6B	0.398 (2)	0.6491 (12)	0.3915 (9)	0.0160*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1A	0.0147 (2)	0.0165 (2)	0.0164 (2)	0.00768 (18)	0.00158 (17)	0.00171 (18)
Cl2A	0.0192 (2)	0.0251 (3)	0.0143 (2)	0.0077 (2)	−0.00299 (18)	−0.00561 (19)
O1A	0.0188 (7)	0.0163 (7)	0.0172 (7)	0.0078 (6)	0.0020 (6)	−0.0021 (6)
O2A	0.0182 (7)	0.0184 (7)	0.0177 (7)	0.0084 (6)	0.0001 (6)	−0.0036 (6)
C1A	0.0174 (10)	0.0143 (9)	0.0181 (10)	0.0060 (8)	0.0036 (8)	0.0031 (8)
C2A	0.0166 (10)	0.0196 (10)	0.0207 (10)	0.0089 (8)	0.0013 (8)	0.0042 (8)
C3A	0.0202 (10)	0.0255 (11)	0.0166 (10)	0.0097 (9)	−0.0037 (8)	0.0014 (8)
C4A	0.0196 (10)	0.0208 (10)	0.0138 (9)	0.0067 (8)	−0.0007 (8)	−0.0015 (8)
N5A	0.0154 (8)	0.0161 (8)	0.0138 (8)	0.0061 (7)	0.0005 (6)	0.0000 (6)
C6A	0.0131 (9)	0.0135 (9)	0.0146 (9)	0.0039 (7)	0.0020 (7)	0.0031 (7)
C7A	0.0137 (9)	0.0125 (9)	0.0154 (9)	0.0042 (7)	0.0033 (7)	0.0026 (7)
C8A	0.0122 (9)	0.0187 (10)	0.0144 (9)	0.0048 (8)	−0.0011 (7)	0.0024 (8)
C9A	0.0150 (9)	0.0151 (9)	0.0121 (9)	0.0016 (8)	0.0004 (7)	−0.0015 (7)

C10A	0.0134 (9)	0.0133 (9)	0.0162 (9)	0.0039 (7)	0.0012 (7)	−0.0005 (7)
N11A	0.0126 (8)	0.0131 (8)	0.0122 (8)	0.0038 (6)	−0.0005 (6)	−0.0011 (6)
C12A	0.0120 (9)	0.0138 (9)	0.0156 (9)	0.0025 (7)	0.0027 (7)	0.0024 (7)
C13A	0.0140 (9)	0.0137 (9)	0.0150 (9)	0.0043 (7)	0.0021 (7)	0.0030 (7)
C14A	0.0145 (9)	0.0116 (9)	0.0147 (9)	0.0046 (7)	0.0028 (7)	0.0010 (7)
C15A	0.0124 (9)	0.0121 (9)	0.0138 (9)	0.0028 (7)	0.0027 (7)	0.0024 (7)
C16A	0.0125 (9)	0.0145 (9)	0.0147 (9)	0.0033 (7)	0.0013 (7)	0.0027 (7)
C17A	0.0133 (9)	0.0130 (9)	0.0148 (9)	0.0034 (7)	0.0014 (7)	0.0028 (7)
Cl1B	0.0148 (2)	0.0186 (2)	0.0217 (2)	0.00967 (18)	0.00275 (18)	0.00399 (19)
Cl2B	0.0183 (2)	0.0231 (3)	0.0153 (2)	0.00847 (19)	−0.00197 (18)	−0.00346 (19)
O1B	0.0201 (7)	0.0182 (7)	0.0213 (7)	0.0103 (6)	0.0049 (6)	0.0004 (6)
O2B	0.0170 (7)	0.0174 (7)	0.0167 (7)	0.0085 (6)	−0.0007 (5)	−0.0024 (6)
C1B	0.0173 (9)	0.0151 (9)	0.0173 (9)	0.0070 (8)	0.0013 (8)	0.0010 (8)
C2B	0.0168 (10)	0.0214 (10)	0.0210 (10)	0.0097 (8)	−0.0012 (8)	0.0028 (8)
C3B	0.0179 (10)	0.0207 (10)	0.0162 (10)	0.0052 (8)	−0.0038 (8)	−0.0006 (8)
C4B	0.0207 (10)	0.0163 (9)	0.0157 (9)	0.0068 (8)	0.0010 (8)	−0.0003 (8)
N5B	0.0162 (8)	0.0149 (8)	0.0153 (8)	0.0059 (7)	0.0022 (6)	0.0011 (7)
C6B	0.0120 (9)	0.0157 (9)	0.0165 (9)	0.0035 (7)	0.0031 (7)	0.0038 (8)
C7B	0.0126 (9)	0.0141 (9)	0.0197 (10)	0.0065 (7)	0.0045 (7)	0.0048 (8)
C8B	0.0148 (9)	0.0190 (10)	0.0156 (9)	0.0057 (8)	−0.0010 (8)	0.0039 (8)
C9B	0.0160 (9)	0.0143 (9)	0.0128 (9)	0.0024 (7)	0.0013 (7)	−0.0001 (7)
C10B	0.0123 (9)	0.0158 (9)	0.0157 (9)	0.0055 (7)	0.0022 (7)	0.0009 (8)
N11B	0.0117 (7)	0.0142 (8)	0.0128 (8)	0.0048 (6)	0.0002 (6)	−0.0001 (6)
C12B	0.0120 (9)	0.0141 (9)	0.0155 (9)	0.0039 (7)	0.0022 (7)	0.0027 (7)
C13B	0.0145 (9)	0.0117 (9)	0.0158 (9)	0.0035 (7)	0.0030 (7)	0.0034 (7)
C14B	0.0141 (9)	0.0126 (9)	0.0166 (9)	0.0053 (7)	0.0049 (7)	0.0022 (7)
C15B	0.0124 (9)	0.0137 (9)	0.0162 (9)	0.0045 (7)	0.0034 (7)	0.0030 (7)
C16B	0.0106 (8)	0.0144 (9)	0.0152 (9)	0.0034 (7)	0.0009 (7)	0.0029 (7)
C17B	0.0145 (9)	0.0137 (9)	0.0144 (9)	0.0045 (7)	0.0024 (7)	0.0034 (7)

Geometric parameters (Å, º)

Cl1A—C7A	1.7272 (19)	C1A—C2A	1.379 (3)
Cl2A—C9A	1.7358 (19)	C1A—H1A	0.937 (15)
Cl1B—C7B	1.7276 (19)	C2A—C3A	1.399 (3)
Cl2B—C9B	1.734 (2)	C2A—H2A	0.929 (16)
O1A—C6A	1.213 (2)	C3A—C4A	1.379 (3)
O2A—C12A	1.221 (2)	C3A—H3A	0.937 (16)
O1B—C6B	1.211 (2)	C4A—C13A	1.399 (3)
O2B—C12B	1.221 (2)	C4A—H4A	0.937 (15)
N5A—C13A	1.405 (2)	C14A—C6A	1.518 (3)
N5A—C14A	1.275 (2)	C15B—C7B	1.387 (3)
N11A—C16A	1.419 (2)	C15B—C16B	1.405 (3)
N11A—C12A	1.396 (2)	C15B—C6B	1.480 (3)
N11A—C14A	1.395 (2)	C7B—C8B	1.387 (3)
N5B—C13B	1.401 (2)	C8B—C9B	1.389 (3)
N5B—C14B	1.277 (3)	C8B—H5B	0.931 (15)
N11B—C16B	1.421 (2)	C9B—C10B	1.390 (3)

N11B—C12B	1.394 (2)	C10B—C16B	1.384 (3)
N11B—C14B	1.396 (2)	C10B—H6B	0.930 (15)
C15A—C7A	1.386 (3)	C12B—C17B	1.467 (3)
C15A—C16A	1.401 (3)	C17B—C1B	1.399 (3)
C15A—C6A	1.477 (3)	C17B—C13B	1.410 (3)
C7A—C8A	1.389 (3)	C1B—C2B	1.378 (3)
C8A—C9A	1.389 (3)	C1B—H1B	0.942 (15)
C8A—H5A	0.925 (15)	C2B—C3B	1.402 (3)
C9A—C10A	1.390 (3)	C2B—H2B	0.947 (16)
C10A—C16A	1.380 (3)	C3B—C4B	1.377 (3)
C10A—H6A	0.938 (15)	C3B—H3B	0.937 (16)
C12A—C17A	1.465 (3)	C4B—C13B	1.399 (3)
C17A—C1A	1.397 (3)	C4B—H4B	0.936 (16)
C17A—C13A	1.412 (3)	C14B—C6B	1.517 (3)
Cl1A—C7A—C15A	121.65 (15)	Cl1B—C7B—C15B	121.43 (15)
Cl1A—C7A—C8A	118.05 (15)	Cl1B—C7B—C8B	118.59 (15)
C15A—C7A—C8A	120.30 (18)	C15B—C7B—C8B	119.98 (18)
C7A—C15A—C6A	132.59 (18)	C7B—C15B—C6B	132.47 (18)
C7A—C15A—C16A	118.79 (17)	C7B—C15B—C16B	118.96 (18)
C6A—C15A—C16A	108.62 (16)	C6B—C15B—C16B	108.54 (16)
C15A—C6A—O1A	129.87 (18)	C15B—C6B—O1B	130.04 (18)
C15A—C6A—C14A	104.37 (15)	C15B—C6B—C14B	104.47 (16)
O1A—C6A—C14A	125.75 (17)	O1B—C6B—C14B	125.46 (18)
C6A—C14A—N5A	126.26 (17)	C6B—C14B—N11B	107.35 (16)
C6A—C14A—N11A	107.38 (16)	C6B—C14B—N5B	126.40 (17)
N5A—C14A—N11A	126.35 (17)	N11B—C14B—N5B	126.25 (17)
C14A—N5A—C13A	115.81 (17)	C14B—N11B—C16B	110.20 (15)
N5A—C13A—C4A	118.48 (17)	C14B—N11B—C12B	122.59 (16)
N5A—C13A—C17A	122.13 (17)	C16B—N11B—C12B	127.14 (16)
C4A—C13A—C17A	119.38 (18)	N11B—C16B—C15B	109.35 (16)
C13A—C4A—C3A	119.69 (19)	N11B—C16B—C10B	127.71 (17)
C13A—C4A—H4A	120.2 (10)	C15B—C16B—C10B	122.94 (18)
C3A—C4A—H4A	120.2 (10)	C16B—C10B—C9B	115.54 (18)
C4A—C3A—C2A	120.96 (19)	C16B—C10B—H6B	122.2 (10)
C4A—C3A—H3A	119.0 (10)	C9B—C10B—H6B	122.3 (10)
C2A—C3A—H3A	120.0 (10)	C10B—C9B—C8B	123.79 (18)
C3A—C2A—C1A	120.04 (19)	C10B—C9B—Cl2B	119.12 (15)
C3A—C2A—H2A	121.2 (10)	C8B—C9B—Cl2B	117.08 (15)
C1A—C2A—H2A	118.8 (10)	C9B—C8B—C7B	118.75 (18)
C2A—C1A—C17A	119.86 (19)	C9B—C8B—H5B	120.6 (10)
C2A—C1A—H1A	119.9 (10)	C7B—C8B—H5B	120.6 (10)
C17A—C1A—H1A	120.2 (10)	N11B—C12B—O2B	121.91 (17)
C13A—C17A—C1A	120.07 (18)	N11B—C12B—C17B	112.41 (16)
C13A—C17A—C12A	120.66 (17)	O2B—C12B—C17B	125.68 (17)
C1A—C17A—C12A	119.26 (17)	C12B—C17B—C13B	120.36 (17)
C17A—C12A—N11A	112.36 (16)	C12B—C17B—C1B	119.93 (17)
C17A—C12A—O2A	125.53 (18)	C13B—C17B—C1B	119.70 (18)

N11A—C12A—O2A	122.11 (17)	C17B—C13B—N5B	122.53 (17)
C12A—N11A—C14A	122.65 (16)	C17B—C13B—C4B	119.38 (18)
C12A—N11A—C16A	127.27 (16)	N5B—C13B—C4B	118.09 (17)
C14A—N11A—C16A	110.08 (15)	C13B—N5B—C14B	115.64 (16)
N11A—C16A—C15A	109.50 (16)	C13B—C4B—C3B	120.22 (19)
N11A—C16A—C10A	127.57 (18)	C13B—C4B—H4B	119.5 (10)
C15A—C16A—C10A	122.93 (18)	C3B—C4B—H4B	120.2 (10)
C16A—C10A—C9A	115.95 (18)	C4B—C3B—C2B	120.39 (19)
C16A—C10A—H6A	122.5 (10)	C4B—C3B—H3B	118.8 (10)
C9A—C10A—H6A	121.5 (10)	C2B—C3B—H3B	120.8 (10)
C10A—C9A—C8A	123.45 (18)	C3B—C2B—C1B	120.12 (19)
C10A—C9A—Cl2A	118.47 (15)	C3B—C2B—H2B	120.2 (10)
C8A—C9A—Cl2A	118.07 (15)	C1B—C2B—H2B	119.6 (10)
C9A—C8A—C7A	118.51 (17)	C17B—C1B—C2B	120.18 (18)
C9A—C8A—H5A	120.8 (10)	C17B—C1B—H1B	120.2 (10)
C7A—C8A—H5A	120.6 (10)	C2B—C1B—H1B	119.6 (10)

Hydrogen-bond geometry (Å, º)

D—H···A	D—H	H···A	D···A	D—H···A
C1B—H1B···Cl1A[i]	0.94 (2)	2.73 (2)	3.637 (2)	162 (1)
C2A—H2A···O1B[ii]	0.93 (2)	2.54 (2)	3.264 (3)	135 (1)
C4B—H4B···N5A[iii]	0.94 (2)	2.56 (2)	3.422 (3)	154 (1)
C10A—H6A···Cl2B[iv]	0.94 (2)	2.67 (2)	3.585 (2)	165 (1)

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