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(5*S*,6*S*,10*R*)-10-(2,4-Dichlorophenyl)-14-[(*E*)-(2,4-dichlorophenyl)methylidene]-3,9-diphenyl-12-[(*R*)-1-phenylethyl]-1,4,7-trioxa-2,8,12-triazadispiro-[4.0.4.4]tetradeca-2,8-diene

S. Mahalakshmi,[a] R. Suresh Kumar,[b] S. Perumal,[b] V. Sivakumar[c] and J. Suresh[c]*

[a]Department of Physics, Madurai Kamaraj University, Madurai 625021, India, [b]School of Chemistry, Madurai Kamaraj University, Madurai 625021, India, and [c]Department of Physics, The Madura College, Madurai 625011, India
Correspondence e-mail: ambujasureshj@yahoo.com

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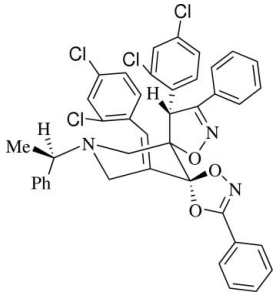
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.013 Å; R factor = 0.044; wR factor = 0.096; data-to-parameter ratio = 8.0.

The asymmetric unit of the title compound, $C_{41}H_{31}Cl_4N_3O_3$, contains two independent molecules with almost identical geometries. The piperidine ring adopts a chair conformation in both molecules, and the dihydroisoxazole rings adopt envelope conformations. The crystal structure is stabilized by C—H···N hydrogen bonds and C—H···π interactions.

Related literature

For related literature, see: Curran (1983); De Amici *et al.* (1990); Diana *et al.* (1985); Faulkner (2001); Gothelf & Jorgensen (1998); Howe & Shelton (1990); Jager & Muller (1985); Kang *et al.* (2000); Konig *et al.* (1990); Kozikowski & Stein (1982); Lepage *et al.* (1992). Martin *et al.* (1989); Nair *et al.* (1999); Padwa (1984); Xue *et al.* (1998).



Experimental

Crystal data

$C_{41}H_{31}Cl_4N_3O_3$
M_r = 755.49
Monoclinic, $P2_1$
a = 13.302 (6) Å
b = 12.551 (9) Å
c = 22.650 (11) Å
β = 105.55 (4)°
V = 3643 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.37 mm^{-1}
T = 293 (2) K
0.25 × 0.18 × 0.13 mm

Data collection

Nonius MACH-3 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.923, T_{max} = 0.953
7698 measured reflections
7370 independent reflections
3074 reflections with $I > 2\sigma(I)$
R_{int} = 0.052
2 standard reflections
frequency: 60 min
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.096
S = 0.99
7370 reflections
921 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}
Absolute structure: Flack (1983), 639 Friedel pairs
Flack parameter: 0.05 (7)

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

D—H···A	D—H	H···A	D···A	D—H···A
C10*B*—H10*D*···N2*B*^{i}	0.96	2.61	3.560 (10)	173
C34*B*—H34*B*···*Cg*1^{ii}	0.93	2.68	3.495 (10)	147
C74*A*—H74*A*···*Cg*2^{iii}	0.93	2.85	3.601 (10)	139

Symmetry codes: (i) $-x, y+\frac{1}{2}, -z$; (ii) $-x+1, y-\frac{1}{2}, -z$; (iii) $x, y-1, z$. *Cg*1 is the centroid of the C91*B*–C96*B* ring. *Cg*2 is the centroid of the ring C12*B*–C17*B* ring.

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; data reduction: *XCAD4* (Harms & Wocadlo, 1996); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2522).

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supplementary materials

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(5*S*,6*S*,10*R*)-10-(2,4-Dichlorophenyl)-14-[(*E*)-(2,4-dichlorophenyl)methylidene]-3,9-diphenyl-12-[(*R*)-1-phenylethyl]-1,4,7-trioxa-2,8,12-triazadispiro[4.0.4.4]tetradeca-2,8-diene

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Comment

1,3-Dipolar cycloaddition reactions afford complex heterocycles with multiple stereocentres, which are useful in the construction of many natural products and pharmaceuticals (Kozikowski & Stein, 1982; Curran, 1983; Jager & Muller, 1985; Martin *et al.*, 1989). 1,3-Dipolar cycloaddition of nitrile oxides to alkenes and α, β -unsaturated carbonyl compounds afford isoxazolines, spiroisoxazolines and dioxazoles (Padwa, 1984; Gothelf & Jorgensen, 1998; Nair *et al.*, 1999). Isoxazolines exhibit antibacterial, antiplatelet, antiviral and anticonvulsant activities, while compounds incorporating spiroisoxazoline sub-structure have stimulated much interest in medicinal and biological chemistry, and hence the structure determination of these compounds is of paramount importance (Diana *et al.*, 1985; De Amici *et al.*, 1990; Howe & Shelton, 1990; Konig *et al.*, 1990; Lepage *et al.*, 1992; Xue *et al.*, 1998; Kang *et al.*, 2000; Faulkner, 2001).

The asymmetric unit of the title compound contains two independent molecules (A and B), with almost identical geometry (Fig.1 and Fig.2). The piperidine ring adopts a chair conformation in both molecules. The olefinic double bonds in molecule A and molecule B have an E configuration and the aryl rings are not coplanar with the adjacent olefinic double bond. The dioxazole ring is essentially planar in both molecules and it forms a dihedral angle of 5.1 (5)° with the attached C12—C17 phenyl ring in molecule A and the corresponding angle is 33.0 (4)° in molecule B. The dihydroisoxazole ring adopts an envelope conformation in both molecules. As a result of steric repulsions the C3—C31—C32 bond angle is widened to 128.5 (8)° in molecule A and 128.6 (8)° in B.

Crystal packing reveals that molecules B are linked by C10B—H10D···N2B (Table 1) hydrogen bonds, generating a C(9) chain along the *b* axis. In addition, weak C—H···π interactions are observed (Table 1).

Experimental

To a solution of 3,5-bis[(*E*)-(2,4-dichlorophenyl)methylidene]-1-[(*R*)-1-phenylethyl]-tetrahydro-4(1*H*)-pyridinone (0.30 g, 0.58 mmol)in benzene (20 ml), benzohydroximoyl chloride (0.316 g, 2.33 mmol) was added and the mixture stirred at room temperature. A solution of triethylamine (0.235 g, 2.33 mmol) in benzene (5 ml) was added dropwise to the above mixture and the stirring was continued for 10 h. The progress of the reaction was monitored by thin-layer chromatography (TLC) with petrolium ether-ethyl acetate (4:1 *v*/*v*) mixture as eluent. After completion of the reaction as evident from TLC, the resulting mixture was filtered to remove the triethylamine hydrochloride, the solvent evaporated *in vacuo* and the residue subjected to flash column chromatography on silica gel (petrolim ether-ethyl acetate, 10:1). The product was recrystallized from ethanol.

Refinement

H atoms were placed at calculated positions and allowed to ride on their carrier atoms with C—H = 0.93–0.98 Å, and U_{iso} = 1.2U_{eq}(C) for CH_2 and CH groups, and 1.5U_{eq} for CH_3 groups. The absolute configuration expected from the starting reagents was confirmed by the refinement of the Flack (1983) parameter.

Figures

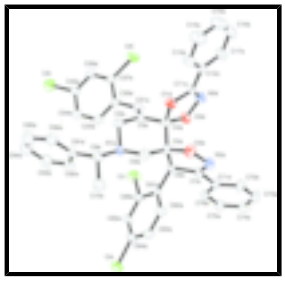


Fig. 1. One of the two independent molecules (molecule A), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 25% probability level. H atoms have been omitted for clarity.

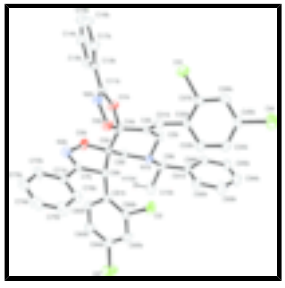


Fig. 2. One of the two independent molecules (molecule B), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 25% probability level. H atoms have been omitted for clarity.

(5*S*,6*S*,10*R*)-10-(2,4-Dichlorophenyl)-14-[(*E*)-(2,4- dichlorophenyl)methylidene]-3,9-diphenyl-12-[(*R*)-1-phenylethyl]- 1,4,7-trioxa-2,8,12-triazadispiro[4.0.4.4]tetradeca-2,8-diene

Crystal data

$C_{41}H_{31}Cl_4N_3O_3$	F_{000} = 1560
M_r = 755.49	D_x = 1.378 Mg m^{-3}
Monoclinic, $P2_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P 2yb	Cell parameters from 25 reflections
a = 13.302 (6) Å	θ = 2–25º
b = 12.551 (9) Å	μ = 0.37 mm^{-1}
c = 22.650 (11) Å	T = 293 (2) K
β = 105.55 (4)º	Needle, colourless
V = 3643 (4) Å^3	0.25 × 0.18 × 0.13 mm
Z = 4	

Data collection

Nonius MACH-3 diffractometer	R_{int} = 0.052
Radiation source: fine-focus sealed tube	θ_{max} = 25.0º
Monochromator: graphite	θ_{min} = 2.1º
T = 293(2) K	h = 0→15
ω–2θ scans	k = −1→14
Absorption correction: ψ scan (North *et al.*, 1968)	l = −26→25
T_{min} = 0.923, T_{max} = 0.953	2 standard reflections

7698 measured reflections
7370 independent reflections
3074 reflections with $I > 2\sigma(I)$

every 60 min
intensity decay: none

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.096$
$S = 0.99$
7370 reflections
921 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0239P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.26$ e Å^{-3}
$\Delta\rho_{min} = -0.22$ e Å^{-3}
Extinction correction: none
Absolute structure: Flack (1983), 639 Friedel pairs
Flack parameter: 0.05 (7)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2$sigma(F^2) is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C2A	0.7448 (6)	0.1884 (6)	0.5804 (3)	0.044 (2)
H2A1	0.7493	0.2417	0.6120	0.053*
H2A2	0.8121	0.1534	0.5879	0.053*
C2B	0.2439 (5)	0.9198 (6)	0.0689 (3)	0.042 (2)
H2B1	0.2436	0.9705	0.1012	0.050*
H2B2	0.3121	0.8863	0.0784	0.050*
C3A	0.6623 (6)	0.1075 (7)	0.5832 (3)	0.041 (2)
C3B	0.1621 (6)	0.8369 (7)	0.0663 (3)	0.039 (2)
C4A	0.5545 (6)	0.1555 (7)	0.5696 (3)	0.046 (2)
C4B	0.0520 (6)	0.8768 (7)	0.0449 (3)	0.045 (2)
C5A	0.5307 (5)	0.2178 (7)	0.5086 (3)	0.043 (2)
C5B	0.0344 (5)	0.9472 (6)	−0.0122 (3)	0.039 (2)
C6A	0.6179 (6)	0.2936 (7)	0.5094 (3)	0.046 (2)

H6A1	0.6029	0.3312	0.4706	0.055*
H6A2	0.6219	0.3459	0.5415	0.055*
C6B	0.1215 (5)	1.0290 (6)	−0.0029 (3)	0.040 (2)
H6B1	0.1105	1.0732	−0.0392	0.049*
H6B2	0.1201	1.0747	0.0314	0.049*
C7A	0.3800 (6)	0.1536 (7)	0.4382 (3)	0.045 (2)
C7B	−0.1079 (6)	0.8727 (7)	−0.0824 (4)	0.042 (2)
C8A	0.4970 (5)	0.1388 (6)	0.4544 (3)	0.037 (2)
H8A	0.5145	0.0661	0.4693	0.044*
C8B	0.0108 (5)	0.8765 (6)	−0.0700 (3)	0.039 (2)
H8B	0.0404	0.8053	−0.0596	0.047*
C9A	0.8018 (6)	0.3189 (7)	0.5168 (4)	0.051 (2)
H9A	0.8080	0.3709	0.5499	0.061*
C9B	0.3081 (6)	1.0556 (7)	0.0103 (4)	0.049 (2)
H9B	0.3075	1.1093	0.0416	0.059*
C10A	0.7746 (6)	0.3782 (7)	0.4560 (4)	0.077 (3)
H10A	0.7125	0.4195	0.4523	0.115*
H10B	0.7630	0.3278	0.4229	0.115*
H10C	0.8311	0.4246	0.4543	0.115*
C10B	0.2886 (6)	1.1112 (7)	−0.0518 (4)	0.070 (3)
H10D	0.2276	1.1552	−0.0584	0.105*
H10E	0.2783	1.0587	−0.0837	0.105*
H10F	0.3478	1.1546	−0.0523	0.105*
C11A	0.4721 (6)	0.1831 (8)	0.6417 (3)	0.047 (2)
C11B	−0.0421 (6)	0.8770 (7)	0.1138 (3)	0.043 (2)
C12A	0.4510 (6)	0.2360 (8)	0.6957 (4)	0.052 (2)
C12B	−0.0760 (6)	0.9107 (8)	0.1653 (4)	0.045 (2)
C13A	0.5074 (7)	0.3262 (9)	0.7204 (4)	0.069 (3)
H13A	0.5554	0.3559	0.7019	0.082*
C13B	−0.0806 (6)	1.0207 (8)	0.1768 (4)	0.067 (3)
H13B	−0.0620	1.0700	0.1509	0.080*
C14A	0.4911 (8)	0.3715 (8)	0.7730 (4)	0.085 (3)
H14A	0.5290	0.4315	0.7900	0.102*
C14B	−0.1127 (6)	1.0549 (9)	0.2265 (4)	0.076 (3)
H14B	−0.1162	1.1276	0.2336	0.092*
C15A	0.4202 (9)	0.3289 (10)	0.8003 (5)	0.089 (4)
H15A	0.4097	0.3592	0.8356	0.107*
C15B	−0.1396 (8)	0.9849 (13)	0.2658 (5)	0.090 (4)
H15B	−0.1598	1.0090	0.2997	0.109*
C16A	0.3662 (8)	0.2431 (10)	0.7751 (5)	0.087 (4)
H16A	0.3168	0.2151	0.7930	0.105*
C16B	−0.1361 (8)	0.8784 (12)	0.2540 (5)	0.096 (4)
H16B	−0.1551	0.8297	0.2800	0.116*
C17A	0.3815 (6)	0.1935 (8)	0.7225 (4)	0.063 (3)
H17A	0.3443	0.1325	0.7066	0.076*
C17B	−0.1049 (6)	0.8417 (8)	0.2040 (4)	0.070 (3)
H17B	−0.1036	0.7688	0.1968	0.084*
C31A	0.6800 (6)	0.0071 (7)	0.5988 (3)	0.046 (2)
H31A	0.6217	−0.0328	0.6000	0.055*

C31B	0.1801 (6)	0.7363 (7)	0.0844 (3)	0.053 (2)
H31B	0.1212	0.6949	0.0820	0.064*
C32A	0.7818 (6)	−0.0515 (7)	0.6149 (4)	0.048 (2)
C32B	0.2813 (6)	0.6817 (6)	0.1076 (4)	0.042 (2)
C33A	0.8438 (7)	−0.0550 (7)	0.5740 (3)	0.057 (3)
H33A	0.8210	−0.0213	0.5362	0.069*
C33B	0.3431 (6)	0.6561 (7)	0.0694 (4)	0.056 (2)
H33B	0.3261	0.6827	0.0296	0.067*
C34A	0.9375 (7)	−0.1072 (7)	0.5887 (4)	0.060 (3)
H34A	0.9795	−0.1072	0.5618	0.073*
C34B	0.4300 (7)	0.5915 (8)	0.0894 (4)	0.068 (3)
H34B	0.4707	0.5735	0.0633	0.082*
C35A	0.9690 (6)	−0.1605 (7)	0.6447 (4)	0.054 (2)
C35B	0.4549 (6)	0.5545 (7)	0.1489 (5)	0.062 (3)
C36A	0.9103 (6)	−0.1583 (6)	0.6848 (4)	0.050 (2)
H36A	0.9330	−0.1926	0.7225	0.060*
C36B	0.3974 (7)	0.5809 (8)	0.1887 (4)	0.058 (2)
H36B	0.4157	0.5571	0.2290	0.070*
C37A	0.8167 (6)	−0.1051 (7)	0.6696 (3)	0.046 (2)
C37B	0.3120 (6)	0.6436 (7)	0.1663 (4)	0.048 (2)
C71A	0.3001 (6)	0.0902 (7)	0.3964 (3)	0.039 (2)
C71B	−0.1767 (6)	0.7966 (7)	−0.1227 (3)	0.043 (2)
C72A	0.1961 (7)	0.1077 (7)	0.3899 (4)	0.056 (2)
H72A	0.1753	0.1619	0.4121	0.067*
C72B	−0.2835 (7)	0.8010 (8)	−0.1312 (4)	0.062 (3)
H72B	−0.3119	0.8517	−0.1104	0.075*
C73A	0.1214 (6)	0.0451 (9)	0.3504 (4)	0.067 (3)
H73A	0.0510	0.0567	0.3468	0.081*
C73B	−0.3483 (7)	0.7300 (9)	−0.1705 (4)	0.072 (3)
H73B	−0.4202	0.7331	−0.1765	0.087*
C74A	0.1507 (7)	−0.0327 (7)	0.3170 (4)	0.056 (2)
H74A	0.1002	−0.0729	0.2897	0.068*
C74B	−0.3051 (9)	0.6547 (9)	−0.2005 (4)	0.078 (3)
H74B	−0.3485	0.6083	−0.2279	0.093*
C75A	0.2542 (7)	−0.0522 (7)	0.3233 (4)	0.056 (3)
H75A	0.2740	−0.1068	0.3011	0.068*
C75B	−0.2008 (8)	0.6473 (8)	−0.1909 (4)	0.073 (3)
H75B	−0.1729	0.5942	−0.2103	0.088*
C76A	0.3291 (6)	0.0088 (7)	0.3627 (3)	0.052 (3)
H76A	0.3994	−0.0045	0.3667	0.062*
C76B	−0.1347 (6)	0.7186 (7)	−0.1520 (4)	0.059 (2)
H76B	−0.0629	0.7137	−0.1457	0.071*
C81A	0.5389 (5)	0.1586 (6)	0.3992 (3)	0.0343 (19)
C81B	0.0419 (6)	0.9192 (7)	−0.1235 (4)	0.043 (2)
C82A	0.5102 (6)	0.2491 (7)	0.3633 (3)	0.050 (2)
H82A	0.4663	0.2989	0.3740	0.060*
C82B	−0.0123 (6)	1.0065 (6)	−0.1562 (4)	0.047 (2)
H82B	−0.0670	1.0364	−0.1436	0.056*
C83A	0.5454 (6)	0.2664 (7)	0.3123 (3)	0.051 (2)

H83A	0.5255	0.3274	0.2888	0.062*
C83B	0.0132 (6)	1.0487 (8)	−0.2060 (4)	0.064 (3)
H83B	−0.0256	1.1051	−0.2272	0.077*
C84A	0.6094 (6)	0.1939 (8)	0.2964 (3)	0.053 (2)
C84B	0.0942 (7)	1.0091 (9)	−0.2247 (4)	0.063 (3)
C85A	0.6396 (6)	0.1031 (7)	0.3295 (3)	0.046 (2)
H85A	0.6819	0.0531	0.3176	0.055*
C85B	0.1506 (7)	0.9227 (8)	−0.1950 (4)	0.062 (3)
H85B	0.2054	0.8941	−0.2081	0.074*
C86A	0.6058 (5)	0.0880 (6)	0.3808 (3)	0.041 (2)
C86B	0.1226 (6)	0.8801 (6)	−0.1448 (3)	0.046 (2)
C91A	0.9062 (6)	0.2626 (7)	0.5259 (4)	0.047 (2)
C91B	0.4147 (6)	1.0043 (7)	0.0253 (4)	0.045 (2)
C92A	0.9181 (7)	0.1753 (8)	0.4907 (4)	0.057 (2)
H92A	0.8602	0.1470	0.4624	0.069*
C92B	0.4330 (7)	0.9131 (7)	−0.0037 (4)	0.054 (2)
H92B	0.3778	0.8776	−0.0304	0.064*
C93A	1.0149 (8)	0.1304 (8)	0.4974 (4)	0.080 (3)
H93A	1.0215	0.0706	0.4744	0.096*
C93B	0.5328 (8)	0.8741 (8)	0.0066 (5)	0.075 (3)
H93B	0.5439	0.8122	−0.0133	0.090*
C94A	1.1030 (8)	0.1734 (10)	0.5381 (5)	0.083 (3)
H94A	1.1684	0.1431	0.5422	0.100*
C94B	0.6155 (9)	0.9233 (10)	0.0450 (5)	0.085 (4)
H94B	0.6824	0.8961	0.0509	0.102*
C95A	1.0924 (8)	0.2594 (10)	0.5714 (5)	0.086 (3)
H95A	1.1510	0.2897	0.5980	0.103*
C95B	0.5995 (7)	1.0142 (9)	0.0755 (4)	0.074 (3)
H95B	0.6552	1.0488	0.1022	0.089*
C96A	0.9953 (7)	0.3029 (8)	0.5665 (4)	0.065 (3)
H96A	0.9894	0.3608	0.5910	0.079*
C96B	0.4992 (7)	1.0529 (7)	0.0654 (4)	0.054 (2)
H96B	0.4881	1.1136	0.0864	0.064*
Cl1	0.64483 (17)	−0.02951 (19)	0.42243 (9)	0.0663 (7)
Cl2	0.19462 (16)	0.7703 (2)	−0.10886 (10)	0.0697 (7)
Cl3	0.24123 (17)	0.6809 (2)	0.21877 (10)	0.0753 (8)
Cl4	0.65079 (16)	0.2120 (2)	0.23013 (9)	0.0729 (8)
Cl5	0.73986 (17)	−0.1046 (2)	0.72106 (9)	0.0732 (8)
Cl6	1.08791 (18)	−0.2274 (2)	0.66324 (10)	0.0768 (8)
Cl7	0.1266 (2)	1.0614 (3)	−0.28807 (11)	0.1020 (10)
Cl8	0.56087 (19)	0.4679 (2)	0.17350 (12)	0.1020 (10)
N1A	0.7191 (5)	0.2401 (5)	0.5198 (3)	0.0442 (18)
N1B	0.2240 (4)	0.9766 (5)	0.0091 (3)	0.0394 (16)
N2A	0.4279 (5)	0.1012 (6)	0.6167 (3)	0.054 (2)
N2B	−0.0751 (4)	0.7926 (6)	0.0825 (3)	0.0460 (18)
N3A	0.3514 (5)	0.2335 (6)	0.4662 (3)	0.054 (2)
N3B	−0.1465 (5)	0.9463 (6)	−0.0560 (3)	0.054 (2)
O1A	0.5491 (4)	0.2254 (4)	0.6190 (2)	0.0480 (15)
O1B	0.0286 (4)	0.9362 (4)	0.0949 (2)	0.0491 (15)

O2A	0.4750 (4)	0.0771 (4)	0.5682 (2)	0.0495 (14)
O2B	−0.0216 (4)	0.7894 (4)	0.0356 (2)	0.0500 (14)
O3A	0.4388 (4)	0.2818 (5)	0.5056 (2)	0.0536 (15)
O3B	−0.0621 (4)	1.0063 (4)	−0.0180 (2)	0.0520 (15)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C2A	0.050 (5)	0.042 (6)	0.038 (5)	−0.003 (5)	0.009 (4)	−0.008 (5)
C2B	0.044 (5)	0.030 (5)	0.054 (5)	−0.009 (4)	0.019 (4)	−0.006 (4)
C3A	0.056 (6)	0.035 (6)	0.035 (5)	−0.004 (5)	0.018 (4)	0.001 (4)
C3B	0.045 (6)	0.037 (6)	0.037 (5)	−0.010 (5)	0.014 (4)	0.000 (4)
C4A	0.052 (6)	0.042 (6)	0.045 (5)	−0.021 (5)	0.016 (5)	−0.015 (5)
C4B	0.038 (5)	0.042 (6)	0.058 (6)	−0.012 (5)	0.019 (4)	−0.021 (5)
C5A	0.038 (5)	0.043 (5)	0.052 (5)	0.004 (5)	0.019 (4)	−0.005 (5)
C5B	0.039 (5)	0.028 (5)	0.049 (5)	0.013 (4)	0.012 (4)	0.002 (4)
C6A	0.057 (6)	0.032 (6)	0.046 (5)	0.002 (5)	0.009 (4)	−0.011 (4)
C6B	0.050 (5)	0.020 (5)	0.054 (5)	−0.011 (4)	0.018 (4)	−0.005 (4)
C7A	0.039 (5)	0.047 (6)	0.051 (5)	0.012 (5)	0.014 (4)	−0.002 (5)
C7B	0.046 (5)	0.028 (5)	0.051 (5)	0.008 (5)	0.012 (4)	0.000 (4)
C8A	0.036 (5)	0.040 (5)	0.034 (4)	0.009 (4)	0.008 (4)	0.002 (4)
C8B	0.033 (5)	0.035 (5)	0.049 (5)	0.010 (4)	0.009 (4)	−0.003 (4)
C9A	0.057 (6)	0.042 (6)	0.059 (6)	−0.009 (5)	0.022 (5)	−0.001 (5)
C9B	0.050 (5)	0.035 (6)	0.069 (6)	−0.014 (5)	0.025 (5)	−0.006 (5)
C10A	0.065 (6)	0.069 (7)	0.101 (8)	0.002 (6)	0.031 (6)	0.039 (6)
C10B	0.063 (6)	0.045 (7)	0.104 (8)	−0.003 (5)	0.023 (5)	0.031 (6)
C11A	0.031 (5)	0.073 (8)	0.041 (5)	−0.006 (5)	0.020 (4)	0.003 (5)
C11B	0.033 (5)	0.055 (7)	0.045 (5)	−0.005 (5)	0.016 (4)	−0.003 (5)
C12A	0.042 (5)	0.069 (8)	0.045 (5)	0.002 (5)	0.013 (5)	0.004 (5)
C12B	0.042 (5)	0.056 (7)	0.041 (5)	−0.009 (5)	0.016 (4)	−0.006 (5)
C13A	0.078 (7)	0.084 (8)	0.052 (6)	0.002 (7)	0.032 (6)	0.004 (6)
C13B	0.067 (7)	0.069 (9)	0.065 (7)	−0.001 (6)	0.020 (6)	−0.008 (6)
C14A	0.111 (9)	0.073 (9)	0.077 (8)	−0.003 (7)	0.037 (7)	−0.017 (7)
C14B	0.060 (7)	0.091 (9)	0.078 (8)	0.024 (6)	0.019 (6)	−0.026 (7)
C15A	0.125 (11)	0.090 (10)	0.067 (7)	0.014 (8)	0.050 (8)	−0.032 (7)
C15B	0.057 (7)	0.165 (15)	0.052 (7)	−0.001 (9)	0.019 (5)	−0.019 (9)
C16A	0.090 (8)	0.108 (11)	0.085 (8)	0.030 (8)	0.060 (7)	0.005 (8)
C16B	0.078 (8)	0.144 (13)	0.084 (9)	−0.037 (9)	0.051 (7)	−0.001 (9)
C17A	0.062 (6)	0.069 (7)	0.068 (6)	0.007 (6)	0.034 (5)	0.008 (6)
C17B	0.066 (7)	0.081 (8)	0.068 (7)	−0.024 (6)	0.027 (6)	−0.009 (6)
C31A	0.063 (6)	0.036 (6)	0.038 (5)	−0.011 (5)	0.011 (4)	0.001 (4)
C31B	0.051 (6)	0.061 (7)	0.047 (5)	−0.014 (5)	0.012 (5)	0.002 (5)
C32A	0.044 (5)	0.053 (7)	0.039 (5)	−0.006 (5)	−0.002 (5)	0.002 (5)
C32B	0.043 (5)	0.027 (5)	0.049 (5)	−0.002 (4)	0.001 (4)	0.005 (4)
C33A	0.066 (6)	0.058 (7)	0.041 (5)	0.000 (6)	0.002 (5)	0.017 (5)
C33B	0.061 (6)	0.051 (6)	0.061 (6)	0.007 (5)	0.026 (5)	0.004 (5)
C34A	0.063 (6)	0.071 (7)	0.049 (6)	−0.002 (6)	0.016 (5)	0.007 (6)
C34B	0.061 (6)	0.078 (8)	0.068 (7)	0.029 (6)	0.023 (5)	−0.008 (6)

C35A	0.060 (6)	0.052 (6)	0.048 (5)	−0.004 (5)	0.011 (5)	0.013 (5)
C35B	0.045 (6)	0.052 (7)	0.086 (7)	0.013 (5)	0.008 (6)	0.003 (6)
C36A	0.065 (6)	0.032 (5)	0.049 (5)	−0.006 (5)	0.008 (5)	0.021 (4)
C36B	0.066 (6)	0.061 (7)	0.045 (5)	−0.009 (6)	0.008 (5)	0.009 (5)
C37A	0.060 (6)	0.043 (6)	0.033 (5)	−0.005 (5)	0.009 (4)	0.000 (5)
C37B	0.044 (5)	0.049 (6)	0.048 (5)	−0.004 (5)	0.010 (4)	0.001 (5)
C71A	0.041 (5)	0.035 (6)	0.042 (5)	0.006 (5)	0.011 (4)	0.011 (5)
C71B	0.034 (5)	0.047 (6)	0.046 (5)	−0.001 (5)	0.006 (4)	0.009 (5)
C72A	0.047 (6)	0.050 (6)	0.070 (6)	0.020 (5)	0.014 (5)	0.008 (5)
C72B	0.047 (6)	0.068 (8)	0.062 (6)	−0.005 (6)	−0.002 (5)	0.013 (6)
C73A	0.037 (6)	0.082 (8)	0.075 (7)	0.000 (6)	0.003 (5)	0.008 (6)
C73B	0.051 (6)	0.094 (10)	0.063 (7)	−0.027 (7)	0.002 (5)	0.029 (6)
C74A	0.067 (7)	0.044 (6)	0.054 (6)	−0.004 (6)	0.009 (5)	−0.008 (5)
C74B	0.088 (9)	0.066 (8)	0.064 (7)	−0.031 (8)	−0.005 (7)	0.012 (6)
C75A	0.059 (6)	0.049 (7)	0.066 (6)	0.008 (6)	0.025 (5)	−0.005 (5)
C75B	0.080 (8)	0.051 (7)	0.076 (7)	−0.010 (7)	−0.001 (6)	−0.001 (6)
C76A	0.035 (5)	0.065 (7)	0.051 (6)	−0.006 (5)	0.004 (5)	−0.008 (5)
C76B	0.054 (6)	0.048 (6)	0.070 (6)	−0.008 (6)	0.007 (5)	−0.004 (6)
C81A	0.031 (4)	0.038 (5)	0.032 (5)	0.005 (4)	0.003 (4)	−0.001 (4)
C81B	0.038 (5)	0.037 (6)	0.056 (6)	0.000 (5)	0.017 (5)	−0.006 (5)
C82A	0.056 (6)	0.046 (7)	0.046 (5)	0.006 (5)	0.013 (5)	−0.007 (5)
C82B	0.056 (6)	0.033 (6)	0.061 (6)	0.003 (5)	0.029 (5)	0.000 (5)
C83A	0.063 (6)	0.046 (6)	0.044 (5)	0.013 (5)	0.012 (5)	0.019 (5)
C83B	0.052 (6)	0.064 (7)	0.073 (7)	−0.004 (6)	0.012 (5)	0.008 (6)
C84A	0.057 (6)	0.064 (7)	0.041 (5)	−0.008 (6)	0.022 (5)	−0.007 (5)
C84B	0.061 (7)	0.073 (9)	0.058 (6)	−0.027 (6)	0.022 (6)	−0.010 (6)
C85A	0.047 (5)	0.049 (6)	0.048 (5)	0.003 (5)	0.024 (4)	−0.002 (5)
C85B	0.056 (6)	0.073 (8)	0.062 (6)	−0.022 (6)	0.025 (5)	−0.032 (6)
C86A	0.044 (5)	0.041 (6)	0.040 (5)	0.010 (5)	0.012 (4)	0.006 (4)
C86B	0.037 (5)	0.042 (6)	0.049 (5)	−0.005 (5)	−0.003 (4)	−0.007 (5)
C91A	0.055 (6)	0.039 (6)	0.054 (6)	−0.002 (5)	0.030 (5)	0.000 (5)
C91B	0.038 (5)	0.044 (6)	0.052 (5)	0.002 (5)	0.012 (5)	0.015 (5)
C92A	0.061 (6)	0.055 (7)	0.060 (6)	−0.001 (6)	0.024 (5)	0.001 (5)
C92B	0.047 (6)	0.041 (6)	0.074 (7)	0.002 (5)	0.016 (5)	0.001 (5)
C93A	0.073 (7)	0.074 (9)	0.105 (9)	0.008 (7)	0.043 (7)	0.011 (7)
C93B	0.077 (7)	0.050 (8)	0.099 (9)	0.004 (7)	0.023 (7)	0.008 (6)
C94A	0.062 (7)	0.093 (10)	0.101 (9)	0.034 (8)	0.032 (7)	0.036 (8)
C94B	0.070 (8)	0.082 (10)	0.107 (10)	0.014 (8)	0.029 (8)	0.036 (8)
C95A	0.057 (7)	0.102 (10)	0.101 (8)	0.001 (7)	0.027 (6)	0.002 (8)
C95B	0.039 (6)	0.097 (10)	0.078 (8)	−0.014 (7)	−0.001 (6)	0.019 (7)
C96A	0.072 (7)	0.067 (8)	0.060 (6)	−0.002 (7)	0.021 (6)	0.006 (6)
C96B	0.056 (6)	0.048 (6)	0.053 (6)	−0.014 (6)	0.007 (5)	0.006 (5)
Cl1	0.0870 (17)	0.0475 (16)	0.0696 (15)	0.0249 (14)	0.0300 (13)	0.0126 (14)
Cl2	0.0575 (14)	0.0606 (17)	0.0890 (17)	0.0147 (14)	0.0160 (13)	−0.0193 (16)
Cl3	0.0742 (16)	0.089 (2)	0.0697 (15)	−0.0038 (16)	0.0318 (13)	−0.0080 (15)
Cl4	0.0707 (15)	0.094 (2)	0.0623 (15)	0.0114 (16)	0.0325 (13)	0.0181 (15)
Cl5	0.0824 (17)	0.085 (2)	0.0567 (15)	0.0028 (16)	0.0262 (14)	0.0154 (15)
Cl6	0.0818 (17)	0.0712 (18)	0.0769 (16)	0.0228 (16)	0.0205 (14)	0.0162 (16)
Cl7	0.127 (2)	0.110 (3)	0.0870 (19)	−0.045 (2)	0.0584 (18)	−0.0013 (18)

Cl8	0.092 (2)	0.091 (2)	0.119 (2)	0.043 (2)	0.0213 (17)	0.018 (2)
N1A	0.039 (4)	0.050 (5)	0.043 (4)	0.008 (4)	0.012 (3)	0.007 (4)
N1B	0.037 (4)	0.034 (4)	0.048 (4)	−0.003 (4)	0.013 (3)	−0.001 (4)
N2A	0.053 (5)	0.060 (6)	0.052 (5)	−0.010 (4)	0.018 (4)	−0.007 (4)
N2B	0.043 (4)	0.044 (5)	0.053 (4)	−0.008 (4)	0.016 (4)	−0.005 (4)
N3A	0.048 (4)	0.058 (6)	0.057 (5)	0.014 (4)	0.014 (4)	−0.004 (4)
N3B	0.052 (5)	0.043 (5)	0.063 (5)	−0.004 (4)	0.009 (4)	0.003 (4)
O1A	0.054 (3)	0.049 (4)	0.045 (3)	−0.008 (3)	0.022 (3)	−0.015 (3)
O1B	0.056 (3)	0.041 (4)	0.057 (4)	−0.020 (3)	0.025 (3)	−0.017 (3)
O2A	0.054 (3)	0.049 (4)	0.049 (3)	−0.014 (3)	0.021 (3)	−0.014 (3)
O2B	0.050 (3)	0.044 (4)	0.059 (3)	−0.012 (3)	0.020 (3)	−0.009 (3)
O3A	0.057 (4)	0.045 (4)	0.057 (4)	0.010 (3)	0.011 (3)	−0.019 (3)
O3B	0.048 (3)	0.039 (4)	0.070 (4)	0.007 (3)	0.018 (3)	−0.004 (3)

Geometric parameters (Å, °)

C2A—N1A	1.474 (8)	C32B—C33B	1.382 (9)
C2A—C3A	1.508 (10)	C33A—C34A	1.368 (9)
C2A—H2A1	0.97	C33A—H33A	0.93
C2A—H2A2	0.97	C33B—C34B	1.385 (10)
C2B—N1B	1.491 (8)	C33B—H33B	0.93
C2B—C3B	1.495 (9)	C34A—C35A	1.394 (10)
C2B—H2B1	0.97	C34A—H34A	0.93
C2B—H2B2	0.97	C34B—C35B	1.380 (11)
C3A—C31A	1.312 (10)	C34B—H34B	0.93
C3A—C4A	1.509 (10)	C35A—C36A	1.348 (9)
C3B—C31B	1.329 (10)	C35A—Cl6	1.740 (8)
C3B—C4B	1.500 (10)	C35B—C36B	1.370 (10)
C4A—O2A	1.438 (8)	C35B—Cl8	1.749 (9)
C4A—O1A	1.438 (8)	C36A—C37A	1.373 (10)
C4A—C5A	1.546 (10)	C36A—H36A	0.93
C4B—O2B	1.447 (8)	C36B—C37B	1.363 (10)
C4B—O1B	1.456 (8)	C36B—H36B	0.93
C4B—C5B	1.532 (9)	C37A—Cl5	1.745 (7)
C5A—O3A	1.449 (8)	C37B—Cl3	1.766 (7)
C5A—C6A	1.496 (9)	C71A—C72A	1.369 (9)
C5A—C8A	1.548 (9)	C71A—C76A	1.391 (10)
C5B—O3B	1.458 (7)	C71B—C76B	1.382 (10)
C5B—C6B	1.520 (9)	C71B—C72B	1.383 (9)
C5B—C8B	1.542 (9)	C72A—C73A	1.389 (10)
C6A—N1A	1.465 (8)	C72A—H72A	0.93
C6A—H6A1	0.97	C72B—C73B	1.386 (11)
C6A—H6A2	0.97	C72B—H72B	0.93
C6B—N1B	1.473 (8)	C73A—C74A	1.355 (11)
C6B—H6B1	0.97	C73A—H73A	0.93
C6B—H6B2	0.97	C73B—C74B	1.377 (12)
C7A—N3A	1.297 (9)	C73B—H73B	0.93
C7A—C71A	1.456 (10)	C74A—C75A	1.368 (9)
C7A—C8A	1.512 (9)	C74A—H74A	0.93

C7B—N3B	1.279 (9)	C74B—C75B	1.348 (11)
C7B—C71B	1.461 (10)	C74B—H74B	0.93
C7B—C8B	1.529 (9)	C75A—C76A	1.377 (9)
C8A—C81A	1.518 (8)	C75A—H75A	0.93
C8A—H8A	0.98	C75B—C76B	1.390 (10)
C8B—C81B	1.482 (9)	C75B—H75B	0.93
C8B—H8B	0.98	C76A—H76A	0.93
C9A—N1A	1.495 (8)	C76B—H76B	0.93
C9A—C10A	1.522 (9)	C81A—C82A	1.389 (10)
C9A—C91A	1.523 (10)	C81A—C86A	1.396 (9)
C9A—H9A	0.98	C81B—C86B	1.379 (9)
C9B—N1B	1.488 (9)	C81B—C82B	1.408 (10)
C9B—C91B	1.511 (10)	C82A—C83A	1.376 (9)
C9B—C10B	1.529 (9)	C82A—H82A	0.93
C9B—H9B	0.98	C82B—C83B	1.369 (10)
C10A—H10A	0.96	C82B—H82B	0.93
C10A—H10B	0.96	C83A—C84A	1.358 (10)
C10A—H10C	0.96	C83A—H83A	0.93
C10B—H10D	0.96	C83B—C84B	1.354 (10)
C10B—H10E	0.96	C83B—H83B	0.93
C10B—H10F	0.96	C84A—C85A	1.365 (11)
C11A—N2A	1.243 (10)	C84A—Cl4	1.747 (8)
C11A—O1A	1.370 (8)	C84B—C85B	1.385 (11)
C11A—C12A	1.482 (11)	C84B—Cl7	1.734 (9)
C11B—N2B	1.285 (9)	C85A—C86A	1.367 (9)
C11B—O1B	1.357 (8)	C85A—H85A	0.93
C11B—C12B	1.422 (10)	C85B—C86B	1.395 (10)
C12A—C17A	1.346 (10)	C85B—H85B	0.93
C12A—C13A	1.389 (11)	C86A—Cl1	1.753 (8)
C12B—C17B	1.359 (11)	C86B—Cl2	1.750 (8)
C12B—C13B	1.409 (11)	C91A—C96A	1.385 (10)
C13A—C14A	1.388 (11)	C91A—C92A	1.390 (11)
C13A—H13A	0.93	C91B—C92B	1.374 (10)
C13B—C14B	1.376 (11)	C91B—C96B	1.383 (10)
C13B—H13B	0.93	C92A—C93A	1.377 (10)
C14A—C15A	1.367 (12)	C92A—H92A	0.93
C14A—H14A	0.93	C92B—C93B	1.375 (10)
C14B—C15B	1.364 (14)	C92B—H92B	0.93
C14B—H14B	0.93	C93A—C94A	1.391 (12)
C15A—C16A	1.335 (13)	C93A—H93A	0.93
C15A—H15A	0.93	C93B—C94B	1.355 (12)
C15B—C16B	1.366 (15)	C93B—H93B	0.93
C15B—H15B	0.93	C94A—C95A	1.346 (13)
C16A—C17A	1.406 (11)	C94A—H94A	0.93
C16A—H16A	0.93	C94B—C95B	1.378 (13)
C16B—C17B	1.387 (12)	C94B—H94B	0.93
C16B—H16B	0.93	C95A—C96A	1.379 (11)
C17A—H17A	0.93	C95A—H95A	0.93
C17B—H17B	0.93	C95B—C96B	1.379 (11)

C31A—C32A	1.498 (10)	C95B—H95B	0.93
C31A—H31A	0.93	C96A—H96A	0.93
C31B—C32B	1.475 (10)	C96B—H96B	0.93
C31B—H31B	0.93	N2A—O2A	1.435 (7)
C32A—C37A	1.376 (9)	N2B—O2B	1.429 (7)
C32A—C33A	1.396 (9)	N3A—O3A	1.400 (7)
C32B—C37B	1.367 (9)	N3B—O3B	1.432 (7)
N1A—C2A—C3A	110.2 (6)	C32A—C33A—H33A	119.5
N1A—C2A—H2A1	109.6	C32B—C33B—C34B	121.1 (8)
C3A—C2A—H2A1	109.6	C32B—C33B—H33B	119.5
N1A—C2A—H2A2	109.6	C34B—C33B—H33B	119.5
C3A—C2A—H2A2	109.6	C33A—C34A—C35A	118.8 (8)
H2A1—C2A—H2A2	108.1	C33A—C34A—H34A	120.6
N1B—C2B—C3B	110.3 (6)	C35A—C34A—H34A	120.6
N1B—C2B—H2B1	109.6	C35B—C34B—C33B	118.5 (8)
C3B—C2B—H2B1	109.6	C35B—C34B—H34B	120.8
N1B—C2B—H2B2	109.6	C33B—C34B—H34B	120.8
C3B—C2B—H2B2	109.6	C36A—C35A—C34A	121.1 (8)
H2B1—C2B—H2B2	108.1	C36A—C35A—Cl6	120.0 (7)
C31A—C3A—C2A	125.3 (8)	C34A—C35A—Cl6	118.9 (7)
C31A—C3A—C4A	122.0 (8)	C36B—C35B—C34B	122.1 (8)
C2A—C3A—C4A	112.7 (7)	C36B—C35B—Cl8	119.1 (8)
C31B—C3B—C2B	125.4 (8)	C34B—C35B—Cl8	118.8 (7)
C31B—C3B—C4B	119.7 (8)	C35A—C36A—C37A	119.3 (7)
C2B—C3B—C4B	114.7 (7)	C35A—C36A—H36A	120.4
O2A—C4A—O1A	104.2 (5)	C37A—C36A—H36A	120.4
O2A—C4A—C3A	112.6 (7)	C37B—C36B—C35B	116.8 (8)
O1A—C4A—C3A	109.2 (6)	C37B—C36B—H36B	121.6
O2A—C4A—C5A	110.6 (6)	C35B—C36B—H36B	121.6
O1A—C4A—C5A	110.2 (6)	C36A—C37A—C32A	121.9 (7)
C3A—C4A—C5A	109.9 (6)	C36A—C37A—Cl5	119.2 (6)
O2B—C4B—O1B	103.0 (5)	C32A—C37A—Cl5	118.9 (7)
O2B—C4B—C3B	111.0 (7)	C36B—C37B—C32B	124.5 (7)
O1B—C4B—C3B	108.3 (6)	C36B—C37B—Cl3	116.3 (7)
O2B—C4B—C5B	111.6 (6)	C32B—C37B—Cl3	119.1 (7)
O1B—C4B—C5B	110.1 (6)	C72A—C71A—C76A	118.7 (8)
C3B—C4B—C5B	112.3 (6)	C72A—C71A—C7A	121.5 (8)
O3A—C5A—C6A	106.9 (7)	C76A—C71A—C7A	119.8 (7)
O3A—C5A—C4A	106.9 (6)	C76B—C71B—C72B	119.6 (8)
C6A—C5A—C4A	109.7 (6)	C76B—C71B—C7B	119.9 (7)
O3A—C5A—C8A	104.9 (6)	C72B—C71B—C7B	120.5 (8)
C6A—C5A—C8A	118.4 (6)	C71A—C72A—C73A	120.4 (8)
C4A—C5A—C8A	109.3 (6)	C71A—C72A—H72A	119.8
O3B—C5B—C6B	106.8 (6)	C73A—C72A—H72A	119.8
O3B—C5B—C4B	107.5 (6)	C71B—C72B—C73B	120.2 (9)
C6B—C5B—C4B	109.5 (6)	C71B—C72B—H72B	119.9
O3B—C5B—C8B	104.0 (5)	C73B—C72B—H72B	119.9
C6B—C5B—C8B	118.7 (6)	C74A—C73A—C72A	120.3 (8)
C4B—C5B—C8B	109.6 (6)	C74A—C73A—H73A	119.8

N1A—C6A—C5A	112.7 (7)	C72A—C73A—H73A	119.8
N1A—C6A—H6A1	109.0	C74B—C73B—C72B	119.3 (9)
C5A—C6A—H6A1	109.0	C74B—C73B—H73B	120.4
N1A—C6A—H6A2	109.0	C72B—C73B—H73B	120.4
C5A—C6A—H6A2	109.0	C73A—C74A—C75A	120.2 (9)
H6A1—C6A—H6A2	107.8	C73A—C74A—H74A	119.9
N1B—C6B—C5B	111.0 (6)	C75A—C74A—H74A	119.9
N1B—C6B—H6B1	109.4	C75B—C74B—C73B	120.9 (10)
C5B—C6B—H6B1	109.4	C75B—C74B—H74B	119.5
N1B—C6B—H6B2	109.4	C73B—C74B—H74B	119.5
C5B—C6B—H6B2	109.4	C74A—C75A—C76A	120.1 (8)
H6B1—C6B—H6B2	108.0	C74A—C75A—H75A	120.0
N3A—C7A—C71A	118.8 (7)	C76A—C75A—H75A	120.0
N3A—C7A—C8A	113.3 (7)	C74B—C75B—C76B	120.5 (10)
C71A—C7A—C8A	128.0 (7)	C74B—C75B—H75B	119.7
N3B—C7B—C71B	120.1 (8)	C76B—C75B—H75B	119.7
N3B—C7B—C8B	114.5 (7)	C75A—C76A—C71A	120.3 (8)
C71B—C7B—C8B	125.3 (7)	C75A—C76A—H76A	119.8
C7A—C8A—C81A	111.2 (6)	C71A—C76A—H76A	119.8
C7A—C8A—C5A	100.0 (6)	C71B—C76B—C75B	119.4 (8)
C81A—C8A—C5A	117.1 (6)	C71B—C76B—H76B	120.3
C7A—C8A—H8A	109.4	C75B—C76B—H76B	120.3
C81A—C8A—H8A	109.4	C82A—C81A—C86A	116.1 (7)
C5A—C8A—H8A	109.4	C82A—C81A—C8A	120.8 (7)
C81B—C8B—C7B	111.2 (6)	C86A—C81A—C8A	123.1 (7)
C81B—C8B—C5B	116.6 (7)	C86B—C81B—C82B	115.4 (7)
C7B—C8B—C5B	98.1 (6)	C86B—C81B—C8B	124.9 (8)
C81B—C8B—H8B	110.1	C82B—C81B—C8B	119.7 (7)
C7B—C8B—H8B	110.1	C83A—C82A—C81A	121.3 (8)
C5B—C8B—H8B	110.1	C83A—C82A—H82A	119.4
N1A—C9A—C10A	111.4 (6)	C81A—C82A—H82A	119.4
N1A—C9A—C91A	110.0 (7)	C83B—C82B—C81B	122.0 (8)
C10A—C9A—C91A	109.7 (6)	C83B—C82B—H82B	119.0
N1A—C9A—H9A	108.6	C81B—C82B—H82B	119.0
C10A—C9A—H9A	108.6	C84A—C83A—C82A	119.7 (8)
C91A—C9A—H9A	108.6	C84A—C83A—H83A	120.2
N1B—C9B—C91B	112.1 (7)	C82A—C83A—H83A	120.2
N1B—C9B—C10B	110.2 (6)	C84B—C83B—C82B	120.6 (9)
C91B—C9B—C10B	108.5 (6)	C84B—C83B—H83B	119.7
N1B—C9B—H9B	108.7	C82B—C83B—H83B	119.7
C91B—C9B—H9B	108.7	C83A—C84A—C85A	121.8 (7)
C10B—C9B—H9B	108.7	C83A—C84A—Cl4	120.3 (8)
C9A—C10A—H10A	109.5	C85A—C84A—Cl4	117.8 (7)
C9A—C10A—H10B	109.5	C83B—C84B—C85B	120.5 (9)
H10A—C10A—H10B	109.5	C83B—C84B—Cl7	121.0 (9)
C9A—C10A—H10C	109.5	C85B—C84B—Cl7	118.4 (8)
H10A—C10A—H10C	109.5	C84A—C85A—C86A	117.8 (7)
H10B—C10A—H10C	109.5	C84A—C85A—H85A	121.1
C9B—C10B—H10D	109.5	C86A—C85A—H85A	121.1

C9B—C10B—H10E	109.5	C84B—C85B—C86B	117.9 (8)
H10D—C10B—H10E	109.5	C84B—C85B—H85B	121.1
C9B—C10B—H10F	109.5	C86B—C85B—H85B	121.1
H10D—C10B—H10F	109.5	C85A—C86A—C81A	123.2 (7)
H10E—C10B—H10F	109.5	C85A—C86A—Cl1	117.1 (6)
N2A—C11A—O1A	117.3 (7)	C81A—C86A—Cl1	119.6 (6)
N2A—C11A—C12A	125.2 (8)	C81B—C86B—C85B	123.5 (8)
O1A—C11A—C12A	117.5 (8)	C81B—C86B—Cl2	119.9 (7)
N2B—C11B—O1B	116.1 (7)	C85B—C86B—Cl2	116.6 (7)
N2B—C11B—C12B	124.2 (8)	C96A—C91A—C92A	117.4 (8)
O1B—C11B—C12B	119.7 (8)	C96A—C91A—C9A	120.5 (8)
C17A—C12A—C13A	120.2 (9)	C92A—C91A—C9A	121.9 (8)
C17A—C12A—C11A	120.0 (9)	C92B—C91B—C96B	117.7 (8)
C13A—C12A—C11A	119.8 (8)	C92B—C91B—C9B	121.6 (8)
C17B—C12B—C13B	118.2 (9)	C96B—C91B—C9B	120.6 (8)
C17B—C12B—C11B	123.0 (9)	C93A—C92A—C91A	120.4 (9)
C13B—C12B—C11B	118.8 (9)	C93A—C92A—H92A	119.8
C12A—C13A—C14A	119.2 (9)	C91A—C92A—H92A	119.8
C12A—C13A—H13A	120.4	C91B—C92B—C93B	120.1 (9)
C14A—C13A—H13A	120.4	C91B—C92B—H92B	120.0
C14B—C13B—C12B	119.6 (10)	C93B—C92B—H92B	120.0
C14B—C13B—H13B	120.2	C92A—C93A—C94A	120.8 (10)
C12B—C13B—H13B	120.2	C92A—C93A—H93A	119.6
C15A—C14A—C13A	120.8 (10)	C94A—C93A—H93A	119.6
C15A—C14A—H14A	119.6	C94B—C93B—C92B	121.8 (10)
C13A—C14A—H14A	119.6	C94B—C93B—H93B	119.1
C15B—C14B—C13B	121.7 (11)	C92B—C93B—H93B	119.1
C15B—C14B—H14B	119.1	C95A—C94A—C93A	119.1 (10)
C13B—C14B—H14B	119.1	C95A—C94A—H94A	120.5
C16A—C15A—C14A	118.7 (10)	C93A—C94A—H94A	120.5
C16A—C15A—H15A	120.7	C93B—C94B—C95B	119.4 (11)
C14A—C15A—H15A	120.7	C93B—C94B—H94B	120.3
C14B—C15B—C16B	118.3 (11)	C95B—C94B—H94B	120.3
C14B—C15B—H15B	120.8	C94A—C95A—C96A	120.6 (11)
C16B—C15B—H15B	120.8	C94A—C95A—H95A	119.7
C15A—C16A—C17A	122.4 (10)	C96A—C95A—H95A	119.7
C15A—C16A—H16A	118.8	C94B—C95B—C96B	118.7 (10)
C17A—C16A—H16A	118.8	C94B—C95B—H95B	120.6
C15B—C16B—C17B	121.2 (11)	C96B—C95B—H95B	120.6
C15B—C16B—H16B	119.4	C95A—C96A—C91A	121.7 (9)
C17B—C16B—H16B	119.4	C95A—C96A—H96A	119.2
C12A—C17A—C16A	118.6 (10)	C91A—C96A—H96A	119.2
C12A—C17A—H17A	120.7	C95B—C96B—C91B	122.2 (9)
C16A—C17A—H17A	120.7	C95B—C96B—H96B	118.9
C12B—C17B—C16B	120.9 (10)	C91B—C96B—H96B	118.9
C12B—C17B—H17B	119.6	C6A—N1A—C2A	109.0 (6)
C16B—C17B—H17B	119.6	C6A—N1A—C9A	110.2 (6)
C3A—C31A—C32A	128.4 (8)	C2A—N1A—C9A	110.1 (6)
C3A—C31A—H31A	115.8	C6B—N1B—C9B	111.1 (6)

C32A—C31A—H31A	115.8	C6B—N1B—C2B	108.1 (5)
C3B—C31B—C32B	128.5 (8)	C9B—N1B—C2B	110.6 (6)
C3B—C31B—H31B	115.7	C11A—N2A—O2A	105.9 (6)
C32B—C31B—H31B	115.7	C11B—N2B—O2B	105.7 (6)
C37A—C32A—C33A	117.7 (8)	C7A—N3A—O3A	110.1 (6)
C37A—C32A—C31A	121.6 (8)	C7B—N3B—O3B	108.3 (6)
C33A—C32A—C31A	120.7 (7)	C11A—O1A—C4A	104.7 (6)
C37B—C32B—C33B	117.0 (7)	C11B—O1B—C4B	106.0 (6)
C37B—C32B—C31B	121.1 (7)	N2A—O2A—C4A	107.9 (5)
C33B—C32B—C31B	121.5 (7)	N2B—O2B—C4B	108.8 (5)
C34A—C33A—C32A	121.1 (8)	N3A—O3A—C5A	109.6 (6)
C34A—C33A—H33A	119.5	N3B—O3B—C5B	108.4 (5)
N1A—C2A—C3A—C31A	126.3 (8)	C8B—C7B—C71B—C72B	−179.4 (7)
N1A—C2A—C3A—C4A	−57.1 (8)	C76A—C71A—C72A—C73A	0.1 (12)
N1B—C2B—C3B—C31B	131.5 (8)	C7A—C71A—C72A—C73A	−179.0 (7)
N1B—C2B—C3B—C4B	−52.6 (8)	C76B—C71B—C72B—C73B	−2.4 (12)
C31A—C3A—C4A—O2A	−7.4 (10)	C7B—C71B—C72B—C73B	178.6 (7)
C2A—C3A—C4A—O2A	176.0 (6)	C71A—C72A—C73A—C74A	−1.2 (13)
C31A—C3A—C4A—O1A	107.9 (8)	C71B—C72B—C73B—C74B	0.6 (12)
C2A—C3A—C4A—O1A	−68.8 (8)	C72A—C73A—C74A—C75A	1.9 (13)
C31A—C3A—C4A—C5A	−131.2 (8)	C72B—C73B—C74B—C75B	1.9 (14)
C2A—C3A—C4A—C5A	52.2 (8)	C73A—C74A—C75A—C76A	−1.5 (13)
C31B—C3B—C4B—O2B	−11.9 (10)	C73B—C74B—C75B—C76B	−2.5 (14)
C2B—C3B—C4B—O2B	171.9 (6)	C74A—C75A—C76A—C71A	0.4 (12)
C31B—C3B—C4B—O1B	100.5 (8)	C72A—C71A—C76A—C75A	0.3 (11)
C2B—C3B—C4B—O1B	−75.7 (8)	C7A—C71A—C76A—C75A	179.5 (7)
C31B—C3B—C4B—C5B	−137.6 (8)	C72B—C71B—C76B—C75B	1.8 (12)
C2B—C3B—C4B—C5B	46.2 (9)	C7B—C71B—C76B—C75B	−179.2 (7)
O2A—C4A—C5A—O3A	68.4 (8)	C74B—C75B—C76B—C71B	0.7 (13)
O1A—C4A—C5A—O3A	−46.3 (8)	C7A—C8A—C81A—C82A	48.5 (10)
C3A—C4A—C5A—O3A	−166.6 (6)	C5A—C8A—C81A—C82A	−65.5 (9)
O2A—C4A—C5A—C6A	−176.1 (6)	C7A—C8A—C81A—C86A	−130.3 (7)
O1A—C4A—C5A—C6A	69.2 (8)	C5A—C8A—C81A—C86A	115.7 (8)
C3A—C4A—C5A—C6A	−51.1 (8)	C7B—C8B—C81B—C86B	−139.2 (8)
O2A—C4A—C5A—C8A	−44.7 (8)	C5B—C8B—C81B—C86B	109.5 (8)
O1A—C4A—C5A—C8A	−159.4 (5)	C7B—C8B—C81B—C82B	41.1 (10)
C3A—C4A—C5A—C8A	80.3 (8)	C5B—C8B—C81B—C82B	−70.2 (9)
O2B—C4B—C5B—O3B	71.4 (7)	C86A—C81A—C82A—C83A	0.7 (11)
O1B—C4B—C5B—O3B	−42.4 (8)	C8A—C81A—C82A—C83A	−178.2 (7)
C3B—C4B—C5B—O3B	−163.2 (6)	C86B—C81B—C82B—C83B	0.5 (11)
O2B—C4B—C5B—C6B	−173.0 (5)	C8B—C81B—C82B—C83B	−179.8 (7)
O1B—C4B—C5B—C6B	73.2 (7)	C81A—C82A—C83A—C84A	0.1 (12)
C3B—C4B—C5B—C6B	−47.6 (8)	C81B—C82B—C83B—C84B	−1.7 (13)
O2B—C4B—C5B—C8B	−41.1 (8)	C82A—C83A—C84A—C85A	0.5 (12)
O1B—C4B—C5B—C8B	−154.9 (5)	C82A—C83A—C84A—Cl4	177.5 (6)
C3B—C4B—C5B—C8B	84.3 (8)	C82B—C83B—C84B—C85B	2.2 (13)
O3A—C5A—C6A—N1A	173.1 (5)	C82B—C83B—C84B—Cl7	179.6 (6)
C4A—C5A—C6A—N1A	57.6 (8)	C83A—C84A—C85A—C86A	−1.8 (12)
C8A—C5A—C6A—N1A	−68.9 (9)	Cl4—C84A—C85A—C86A	−178.9 (6)

O3B—C5B—C6B—N1B	174.9 (5)	C83B—C84B—C85B—C86B	−1.4 (12)
C4B—C5B—C6B—N1B	58.8 (8)	Cl7—C84B—C85B—C86B	−178.9 (6)
C8B—C5B—C6B—N1B	−68.1 (8)	C84A—C85A—C86A—C81A	2.7 (12)
N3A—C7A—C8A—C81A	−114.3 (7)	C84A—C85A—C86A—Cl1	179.6 (6)
C71A—C7A—C8A—C81A	65.6 (10)	C82A—C81A—C86A—C85A	−2.1 (11)
N3A—C7A—C8A—C5A	10.0 (8)	C8A—C81A—C86A—C85A	176.8 (7)
C71A—C7A—C8A—C5A	−170.0 (7)	C82A—C81A—C86A—Cl1	−179.0 (5)
O3A—C5A—C8A—C7A	−13.7 (7)	C8A—C81A—C86A—Cl1	−0.1 (10)
C6A—C5A—C8A—C7A	−132.7 (7)	C82B—C81B—C86B—C85B	0.2 (11)
C4A—C5A—C8A—C7A	100.7 (6)	C8B—C81B—C86B—C85B	−179.4 (7)
O3A—C5A—C8A—C81A	106.5 (7)	C82B—C81B—C86B—Cl2	−178.9 (5)
C6A—C5A—C8A—C81A	−12.5 (10)	C8B—C81B—C86B—Cl2	1.4 (10)
C4A—C5A—C8A—C81A	−139.1 (6)	C84B—C85B—C86B—C81B	0.2 (12)
N3B—C7B—C8B—C81B	−104.0 (8)	C84B—C85B—C86B—Cl2	179.4 (6)
C71B—C7B—C8B—C81B	73.3 (10)	N1A—C9A—C91A—C96A	−132.5 (7)
N3B—C7B—C8B—C5B	18.7 (8)	C10A—C9A—C91A—C96A	104.6 (8)
C71B—C7B—C8B—C5B	−164.0 (7)	N1A—C9A—C91A—C92A	53.1 (9)
O3B—C5B—C8B—C81B	94.4 (7)	C10A—C9A—C91A—C92A	−69.8 (9)
C6B—C5B—C8B—C81B	−24.0 (10)	N1B—C9B—C91B—C92B	47.5 (10)
C4B—C5B—C8B—C81B	−150.9 (6)	C10B—C9B—C91B—C92B	−74.4 (9)
O3B—C5B—C8B—C7B	−24.3 (7)	N1B—C9B—C91B—C96B	−137.5 (7)
C6B—C5B—C8B—C7B	−142.7 (7)	C10B—C9B—C91B—C96B	100.6 (8)
C4B—C5B—C8B—C7B	90.5 (7)	C96A—C91A—C92A—C93A	1.3 (11)
N2A—C11A—C12A—C17A	2.1 (13)	C9A—C91A—C92A—C93A	175.8 (8)
O1A—C11A—C12A—C17A	−175.4 (7)	C96B—C91B—C92B—C93B	−1.3 (12)
N2A—C11A—C12A—C13A	178.6 (9)	C9B—C91B—C92B—C93B	173.8 (8)
O1A—C11A—C12A—C13A	1.1 (11)	C91A—C92A—C93A—C94A	−2.0 (13)
N2B—C11B—C12B—C17B	31.9 (13)	C91B—C92B—C93B—C94B	−0.1 (14)
O1B—C11B—C12B—C17B	−148.9 (8)	C92A—C93A—C94A—C95A	0.5 (15)
N2B—C11B—C12B—C13B	−147.8 (9)	C92B—C93B—C94B—C95B	1.0 (15)
O1B—C11B—C12B—C13B	31.4 (11)	C93A—C94A—C95A—C96A	1.5 (15)
C17A—C12A—C13A—C14A	0.1 (13)	C93B—C94B—C95B—C96B	−0.4 (15)
C11A—C12A—C13A—C14A	−176.3 (8)	C94A—C95A—C96A—C91A	−2.3 (14)
C17B—C12B—C13B—C14B	0.6 (13)	C92A—C91A—C96A—C95A	0.8 (12)
C11B—C12B—C13B—C14B	−179.7 (7)	C9A—C91A—C96A—C95A	−173.8 (8)
C12A—C13A—C14A—C15A	−0.5 (15)	C94B—C95B—C96B—C91B	−1.0 (14)
C12B—C13B—C14B—C15B	0.6 (14)	C92B—C91B—C96B—C95B	1.8 (12)
C13A—C14A—C15A—C16A	−0.3 (17)	C9B—C91B—C96B—C95B	−173.3 (8)
C13B—C14B—C15B—C16B	−1.3 (16)	C5A—C6A—N1A—C2A	−62.1 (8)
C14A—C15A—C16A—C17A	1.5 (17)	C5A—C6A—N1A—C9A	177.0 (6)
C14B—C15B—C16B—C17B	0.8 (18)	C3A—C2A—N1A—C6A	59.9 (8)
C13A—C12A—C17A—C16A	1.0 (13)	C3A—C2A—N1A—C9A	−179.1 (6)
C11A—C12A—C17A—C16A	177.4 (8)	C10A—C9A—N1A—C6A	−56.6 (8)
C15A—C16A—C17A—C12A	−1.9 (15)	C91A—C9A—N1A—C6A	−178.5 (6)
C13B—C12B—C17B—C16B	−1.1 (14)	C10A—C9A—N1A—C2A	−176.9 (6)
C11B—C12B—C17B—C16B	179.2 (8)	C91A—C9A—N1A—C2A	61.3 (8)
C15B—C16B—C17B—C12B	0.4 (16)	C5B—C6B—N1B—C9B	172.8 (6)
C2A—C3A—C31A—C32A	−2.4 (13)	C5B—C6B—N1B—C2B	−65.7 (7)
C4A—C3A—C31A—C32A	−178.6 (7)	C91B—C9B—N1B—C6B	177.5 (6)

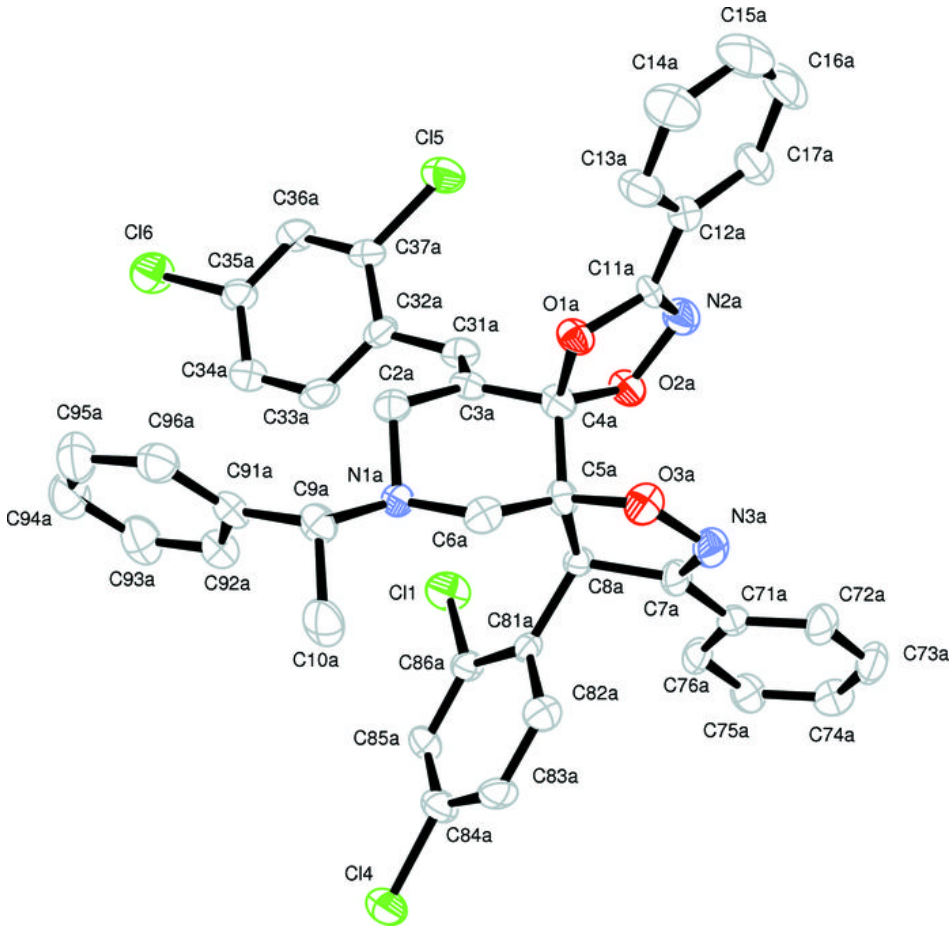
C2B—C3B—C31B—C32B	−3.3 (14)	C10B—C9B—N1B—C6B	−61.5 (8)
C4B—C3B—C31B—C32B	−179.1 (7)	C91B—C9B—N1B—C2B	57.4 (8)
C3A—C31A—C32A—C37A	124.6 (9)	C10B—C9B—N1B—C2B	178.4 (6)
C3A—C31A—C32A—C33A	−56.6 (12)	C3B—C2B—N1B—C6B	60.9 (7)
C3B—C31B—C32B—C37B	115.8 (10)	C3B—C2B—N1B—C9B	−177.2 (6)
C3B—C31B—C32B—C33B	−71.7 (12)	O1A—C11A—N2A—O2A	−0.7 (10)
C37A—C32A—C33A—C34A	−2.0 (13)	C12A—C11A—N2A—O2A	−178.2 (7)
C31A—C32A—C33A—C34A	179.2 (8)	O1B—C11B—N2B—O2B	0.6 (9)
C37B—C32B—C33B—C34B	2.3 (12)	C12B—C11B—N2B—O2B	179.8 (7)
C31B—C32B—C33B—C34B	−170.5 (8)	C71A—C7A—N3A—O3A	178.1 (6)
C32A—C33A—C34A—C35A	2.2 (13)	C8A—C7A—N3A—O3A	−2.0 (9)
C32B—C33B—C34B—C35B	−1.2 (14)	C71B—C7B—N3B—O3B	178.0 (6)
C33A—C34A—C35A—C36A	−2.1 (13)	C8B—C7B—N3B—O3B	−4.6 (9)
C33A—C34A—C35A—Cl6	179.7 (7)	N2A—C11A—O1A—C4A	−0.3 (9)
C33B—C34B—C35B—C36B	−0.9 (15)	C12A—C11A—O1A—C4A	177.4 (7)
C33B—C34B—C35B—Cl8	177.1 (7)	O2A—C4A—O1A—C11A	1.0 (7)
C34A—C35A—C36A—C37A	1.7 (13)	C3A—C4A—O1A—C11A	−119.5 (7)
Cl6—C35A—C36A—C37A	179.9 (6)	C5A—C4A—O1A—C11A	119.7 (6)
C34B—C35B—C36B—C37B	1.7 (14)	N2B—C11B—O1B—C4B	−4.7 (9)
Cl8—C35B—C36B—C37B	−176.3 (7)	C12B—C11B—O1B—C4B	176.0 (7)
C35A—C36A—C37A—C32A	−1.6 (13)	O2B—C4B—O1B—C11B	6.5 (7)
C35A—C36A—C37A—Cl5	178.8 (6)	C3B—C4B—O1B—C11B	−111.1 (7)
C33A—C32A—C37A—C36A	1.6 (12)	C5B—C4B—O1B—C11B	125.7 (6)
C31A—C32A—C37A—C36A	−179.5 (8)	C11A—N2A—O2A—C4A	1.3 (8)
C33A—C32A—C37A—Cl5	−178.7 (6)	O1A—C4A—O2A—N2A	−1.4 (7)
C31A—C32A—C37A—Cl5	0.2 (11)	C3A—C4A—O2A—N2A	116.7 (6)
C35B—C36B—C37B—C32B	−0.4 (13)	C5A—C4A—O2A—N2A	−119.8 (6)
C35B—C36B—C37B—Cl3	−177.8 (7)	C11B—N2B—O2B—C4B	3.9 (8)
C33B—C32B—C37B—C36B	−1.5 (12)	O1B—C4B—O2B—N2B	−6.4 (7)
C31B—C32B—C37B—C36B	171.3 (8)	C3B—C4B—O2B—N2B	109.3 (6)
C33B—C32B—C37B—Cl3	175.8 (6)	C5B—C4B—O2B—N2B	−124.5 (6)
C31B—C32B—C37B—Cl3	−11.4 (11)	C7A—N3A—O3A—C5A	−8.0 (8)
N3A—C7A—C71A—C72A	−5.4 (11)	C6A—C5A—O3A—N3A	140.4 (6)
C8A—C7A—C71A—C72A	174.7 (7)	C4A—C5A—O3A—N3A	−102.1 (6)
N3A—C7A—C71A—C76A	175.5 (7)	C8A—C5A—O3A—N3A	13.9 (7)
C8A—C7A—C71A—C76A	−4.4 (12)	C7B—N3B—O3B—C5B	−13.1 (8)
N3B—C7B—C71B—C76B	178.8 (7)	C6B—C5B—O3B—N3B	150.8 (5)
C8B—C7B—C71B—C76B	1.6 (12)	C4B—C5B—O3B—N3B	−91.8 (6)
N3B—C7B—C71B—C72B	−2.2 (11)	C8B—C5B—O3B—N3B	24.4 (7)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C10B—H10D···N2B^{i}	0.96	2.61	3.560 (10)	173
C34B—H34B···Cg1^{ii}	0.93	2.68	3.495 (10)	147
C74A—H74A···Cg2^{iii}	0.93	2.85	3.601 (10)	139

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

Fig. 1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C14a
C16a
Cl5
C13a
C17a
C36a
Cl6
C37a
C12a
C35a
C11a
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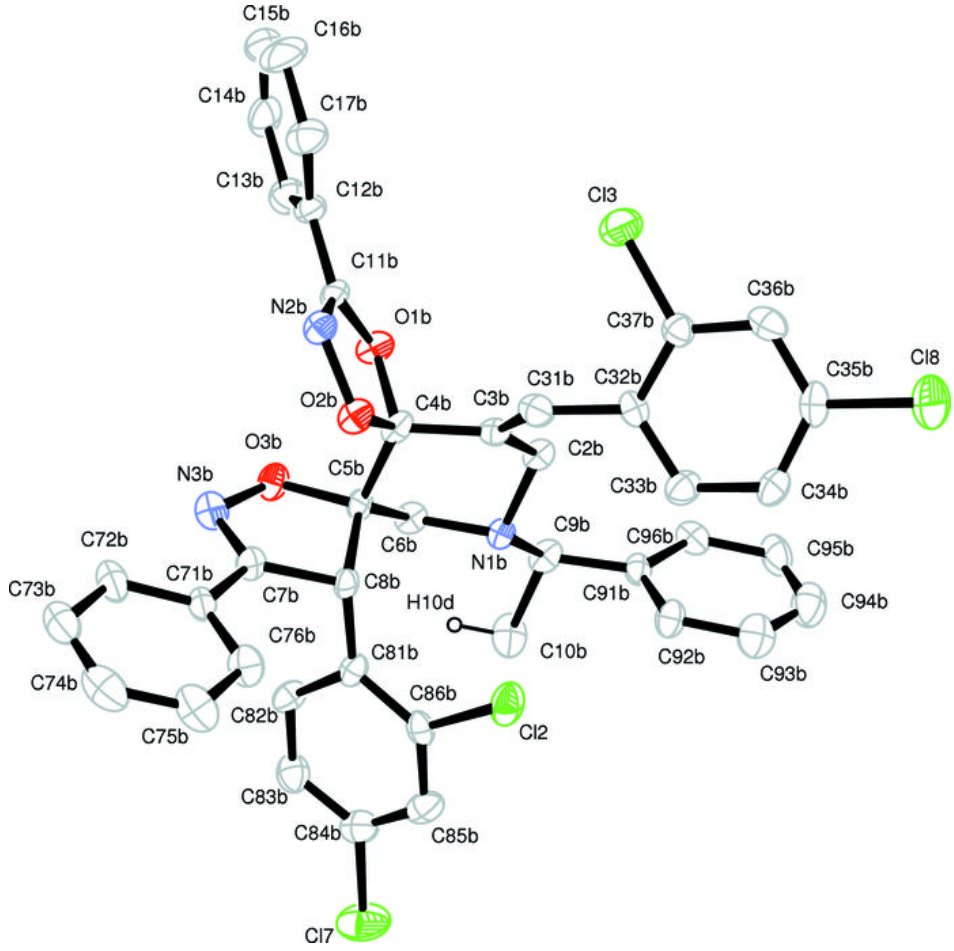
N2a
C31a
C34a
C2a
O2a
C33a
C3a
C4a
C95a
C96a
C91a
N1a
C5a
O3a
C9a
C94a
C6a
N3a
C93a
C92a
Cl1
C8a
C71a
C72a
C7a
C81a
C73a
C10a
C86a
C76a
C82a
C85a
C75a
C74a
C83a
C84a
Cl4

Fig. 2


C15b
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C14b
C17b
C13b
C12b
C11b
N2b
O1b
O2b
C4b
C3b
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C32b
Cl3
C36b
C37b
C35b
Cl8
C2b
O3b
N3b
C5b
C33b
C34b
C72b
C6b
C9b
C96b
C95b
C71b
N1b
C73b
C7b
C8b
H10d
C91b
C94b
C76b
C81b
C10b
C92b
C93b
C74b
C86b
C82b
Cl2
C75b
C83b
C84b
C85b
Cl7