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Crystal structure of 2,2″-bis(2,7-dichloro-9-hydroxy-9*H*-fluoren-9-yl)-1,1′:4′,1″-terphenyl triethylamine trisolvate

Henrik Klien, Wilhelm Seichter and Edwin Weber*

Institut für Organische Chemie, TU Bergakademie Freiberg, Leipziger Strasse 29, D-09596 Freiberg/Sachsen, Germany. *Correspondence e-mail: edwin.weber@chemie-tu.freiberg.de

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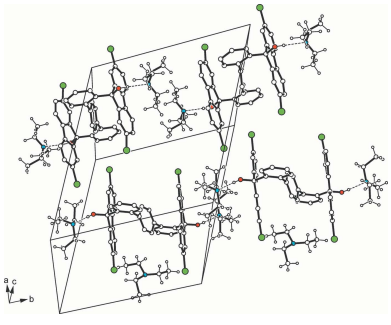
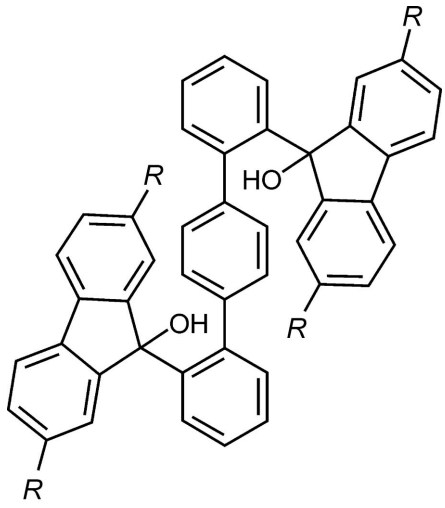
In the title solvate, $C_{44}H_{26}Cl_4O_2\cdot 3C_6H_{15}N$, the asymmetric part of the unit cell comprises two halves of the diol molecules, 2,2″-bis(2,7-dichloro-9-hydroxy-9*H*-fluoren-9-yl)-1,1′:4′,1″-terphenyl, and three molecules of triethylamine, *i. e*. the diol molecules are located on crystallographic symmetry centres. Two of the solvent molecules are disordered over two positions [occupancy ratios of 0.567 (3):0.433 (3) and 0.503 (3):0.497 (3)]. In the diol molecules, the outer rings of the 1,1′:4′,1″-terphenyl elements are twisted with reference to their central arene ring and the mean planes of the fluorenyl moieties are inclined with respect to the terphenyl ring to which they are connected, the latter making dihedral angles of 82.05 (8) and 82.28 (8)°. The presence of two 9-fluoren-9-ol units attached at positions 2 and 2″ of the terphenyl moiety induces a 'folded' geometry which is stabilized by intramolecular C—H···O hydrogen bonds and π–π stacking interactions, the latter formed between the fluorenyl units and the central ring of the terphenyl unit [centroid–centroid distances = 3.559 (1) and 3.562 (1) Å]. The crystal is composed of 1:2 complex units, in which the solvent molecules are associated with the diol molecules *via* O—H···N hydrogen bonds, while the remaining solvent molecule is linked to the host by a C—H···N hydrogen bond. The given pattern of intermolecular interactions results in formation of chain structures extending along [010].

1. Chemical context

Compounds featuring two bulky 9-hydroxy-9-fluorenyl moieties laterally attached to a linear central unit such as a biphenyl group (Weber *et al.*, 1993; Barbour *et al.*, 1993; Ibragimov *et al.*, 2001; Skobridis *et al.*, 2007) or other linear combinations of phenylene and ethylene components (Weber *et al.*, 2002) are well known for their high ability to form crystalline host–guest inclusions (Weber, 1996). Both exchange of the central biphenyl axis for a 1,1′:4′,1″-terphenyl moiety [*cf.* (I)] (Klien *et al.*, 2013, 2014) as well as the addition of substituents to the lateral fluorenyl groups in a representative molecule (Bourne *et al.*, 1994; Caira *et al.*, 1997; Weber *et al.*, 2002) have been performed in order to exercise potential control of the molecular packing in the crystal and thus on the inclusion behavior towards selected guests. Along these lines, aside from conventional hydrogen bonding (Braga & Grepioni, 2004), Cl···Cl supramolecular interactions (Awwadi *et al.*, 2006) have recently been found to support crystal engineering of an intended lattice structure (Metrangolo *et al.*, 2008; Mukherjee *et al.*, 2014). Being associated with this, a corresponding structural modification of the parent molecule (I) by chloro substitution, giving rise to compound (II), presented a promising study. Hence, the synthesis of (II) was undertaken and is reported on here in detail. We were also



successful in preparing a crystalline inclusion solvate of (II) with triethylamine, the title compound (II*a*), the crystal structure of which is described and discussed and compared to the structures of related compounds.



(I) R = H
(II) R = Cl
(II*a*) R = (II)·3Et$_3$N

2. Structural commentary

The title solvate (II*a*) crystallizes in the space group $P\overline{1}$ with two halves of the diol molecules (centred at $x+\frac{1}{2}, y, z$ and $x+1$, $y+\frac{1}{2}, z+\frac{1}{2}$) and three molecules of triethylamine in the asymmetric unit, *i.e.* the diol molecules occupy crystallographic inversion centres (Fig. 1). Two of the solvent molecules are disordered over two positions with occupancy ratios of 0.567 (3):0.433 (3) and 0.503 (3):0.497 (3). A perspective view of the molecular structure including ring specification is depicted in Fig. 1. The fluorenyl moieties of the diol molecules show a slight distortion from strict planarity with the largest distances from the best plane being 0.027 (1) and −0.030 (1) Å for C7 and C10, respectively, and 0.059 (1) and −0.068 (1) Å for C8*A* and C11*A*. respectively The molecules adopt a 'folded' geometry which is stabilized by two types of intermolecular interactions. The OH oxygen atoms form relatively strong C—H···O hydrogen bonds [d(H···O) 2.22, 2.23 Å] (Desiraju & Steiner, 1999) which enforce a nearly orthogonal orientation of the fluorenyl moieties with respect to the terphenyl ring, to which they are attached: the dihedral angles between the five-membered ring of the fluorenyl unit defined by C1–C13 (or C1*A*–C13*A*) and the six-membered rings of the terphenyl unit defined by C14–C19 (or C14*A*–C19*A*) are 82.05 (8) or 82.28 (8)°, respectively. Moreover, the location of the central ring of the terphenyl unit between the fluorenyl units [ring centroid distances = 3.559 (1) and 3.562 (1) Å] indicate the presence of π–π stacking interactions (James, 2004; Martinez & Iverson, 2012) between these molecular parts. These cooperative intramolecular interactions enforce a nearly orthogonal arrangement of the outer ring (*B* or *B*′) with respect to the inner ring (*A* or *A*′) (Fig. 2) of the terphenyl unit [inter-ring dihedral angles = 76.3 (1) and 79.3 (1)°, respectively].

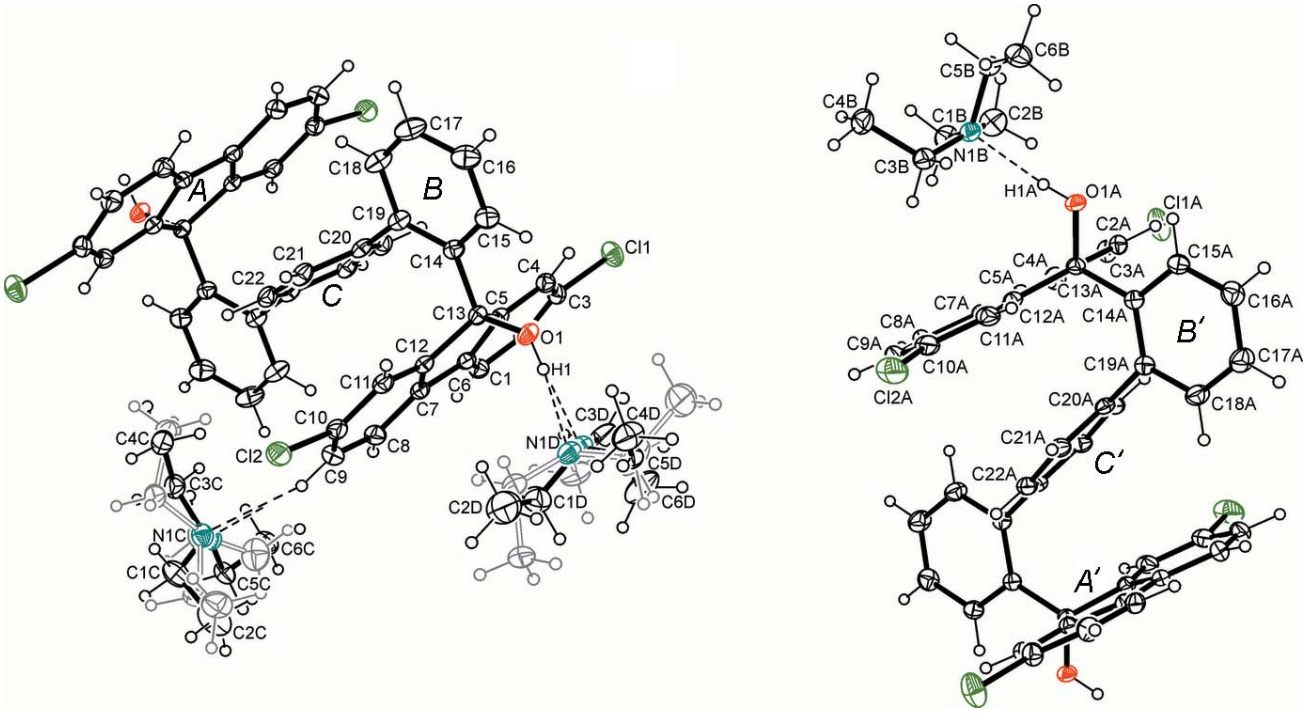


Figure 1
A perspective view of the title solvate (II*a*) including the atom numbering and ring specification. Anisotropic displacement parameters for non-hydrogen atoms are drawn at the 50% probability level. Dashed lines represent hydrogen-bonding interactions. The molecules occupy the symmetry centers $x+\frac{1}{2}$, y, z and $x+1$, $y+\frac{1}{2}$, $z+\frac{1}{2}$)

3. Supramolecular features

According to the distinct acceptor character of the solvent species, the crystal structure is constructed of 1:2 complex units with the nitrogen atom of the solvent hydrogen-bonded to the OH hydrogen atom of the diol host [d(H···N) 1.91–1.95 Å] (Table 1). The remaining solvent molecule is connected to the host *via* C—H···O hydrogen bonding [d(H···N) 2.54; 2.60 Å], giving an overall chain structure extending along [010] (Fig. 2). Interactions involving the chlorine atoms are not perceptible. A comparative consideration regarding the geometric features of the diol molecule in the present structure and the solvent-free structure of the corresponding unsubstituted compound (I) and its derivatives bearing alkyl groups in the 2- and 7-positions of the fluorenyl moieties as well as a variety of their inclusion structures (Klien *et al.* 2013, 2014), reveals restricted conformational flexibility. This means that neither the presence of substituents nor the nature of the included solvent species markedly affect the conformation of the diol molecule. Obviously, the molecular geometries in the solid-state structures follow close-packing requirements and, to a lesser extent, association effects.

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1D^{i}	0.84	1.95	2.781 (2)	171
O1—H1···N1DA^{i}	0.84	1.91	2.731 (2)	164
O1A—H1A···N1B^{ii}	0.84	1.94	2.766 (2)	167
C4—H4···O1A^{iii}	0.95	2.54	3.489 (2)	175
C4A—H4A···O1^{iv}	0.95	2.47	3.403 (2)	168
C9—H9···N1C^{v}	0.95	2.54	3.459 (2)	163
C9—H9···N1CA^{v}	0.95	2.60	3.519 (2)	162

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

4. Database survey

A search of the Cambridge Structural Database (Groom & Allen, 2014) for the 2,2′′-disubstituted *p*-terphenyls yielded eleven hits, namely 4,4′′′′-bis(4-methoxybenzoyl)-1,1′:2′,1′′:4′′,1′′′:2′′′,1′′′′-quinquephenyl (Debroy *et al.*, 2009), 2,2′′-bis(bromomethyl)-*p*-terphenyl (Jones & Kuś, 2005), 2,2′′-dimethyl-*p*-terphenyl (Lunazzi *et al.*, 2005), 2′,4′′,2′′′-quinquephenyl (Toussaint, 1966), 9,9′-(1,1′:4′,1′′-terphenyl-2,2′′-diyl)bis(9*H*-fluorene-9-ol) bis(diethylamine) clathrate (Klien *et al.*, 2013), 9,9′-(1,1′:4′,1′′-terphenyl-2,2′′-diyl)bis(9*H*-fluorene-9-ol) bis(propan-1-ol) clathrate (Klien *et al.*, 2013), 9,9′-(1,1′:4′,1′′-terphenyl-2,2′′-diyl)bis(9*H*-fluorene-9-ol) bis(butan-1-ol) clathrate (Klien *et al.*, 2013), 9,9′-(1,1′:4′,1′′-terphenyl-2,2′′-diyl)bis(9*H*-fluorene-9-ol) bis(ethanol) clathrate (Klien *et al.*, 2013), 9,9′-(1,1′:4′,1′′-terphenyl-2,2′′-diyl)bis(2,7-di-*t*-butyl-9*H*-fluorene-9-ol) bis(propan-1-ol) clathrate (Klien *et al.*, 2013), 9,9′-(1,1′:4′,1′′-terphenyl-2,2′′-diyl)bis(2,7-di-*t*-butyl-9*H*-fluorene-9-ol) bis(diethylamine) clathrate (Klien *et al.*, 2013), 9,9′-(1,1′:4′,1′′-terphenyl-2,2′′-diyl)bis(2,7-di-*t*-butyl-9*H*-fluor-

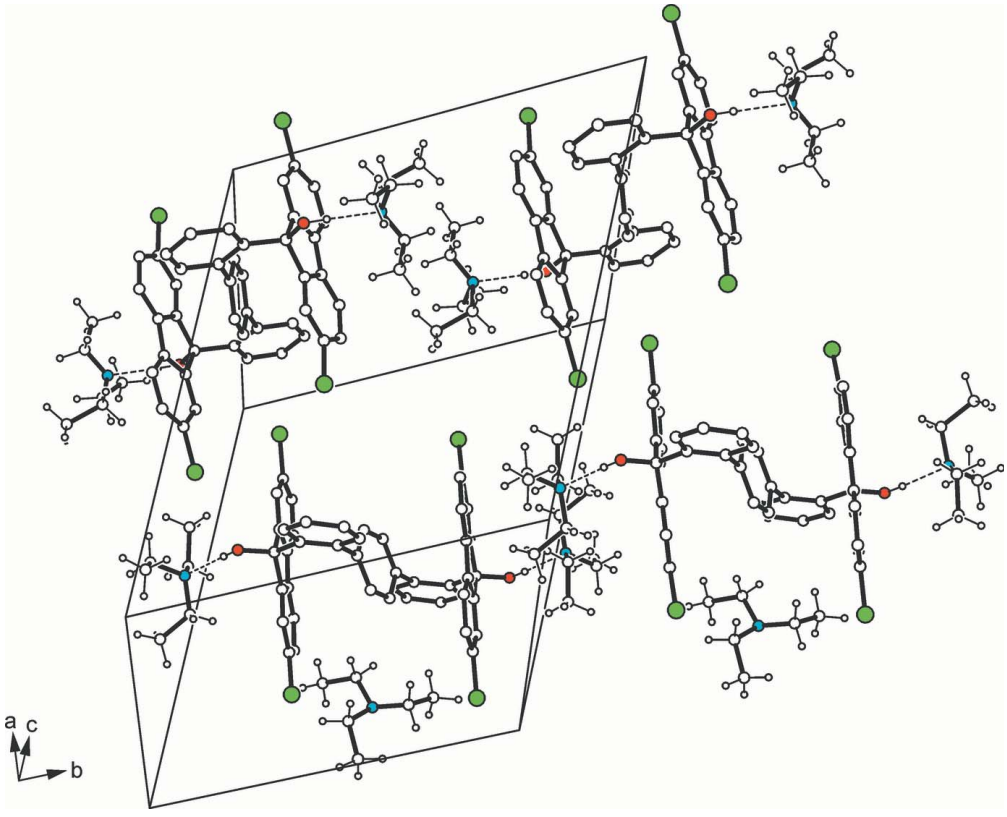


Figure 2
The packing of the title compound (II*a*) in the unit cell. Hydrogen bonds are shown as dashed lines.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{44}H_{26}Cl_4O_2{\cdot}3C_6H_{15}N$
M_r	1032.01
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	100
a, b, c (Å)	14.5995 (2), 14.8094 (2), 15.7705 (3)
α, β, γ (°)	68.373 (1), 66.837 (1), 67.558 (1)
V (Å^3)	2800.13 (8)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.26
Crystal size (mm)	0.42 × 0.40 × 0.23
Data collection	
Diffractometer	Bruker CCD area detector
Absorption correction	Multi-scan (*SADABS*; Bruker, 2008)
T_{min}, T_{max}	0.900, 0.943
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	53831, 14031, 11477
R_{int}	0.025
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.669
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.040, 0.113, 1.01
No. of reflections	14031
No. of parameters	773
No. of restraints	24
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.59, −0.59

Computer programs: *APEX2* and *SAINT* (Bruker, 2008), *SHELXS97* and *SHELXTL* (Sheldrick, 2008), *SHELXL2013* (Sheldrick, 2015) and *ORTEP-3 for Windows* (Farrugia, 2012).

ene-9-ol) bis(butan-1-ol) clathrate (Klien *et al.*, 2013). In all cases, the terphenyl framework adopts a twisted conformation, which in the case of the bisfluorenyl-substituted derivatives is stabilized by intramolecular π–π arene stacking and C—H···O hydrogen bonds. The crystal structures of the clathrates, which involve protic guest species in general, are constructed of 1:2 host–guest complexes with the complex components associated with other *via* O—H···O and O—H···N hydrogen bonds. Both of these features, regarding molecular conformation and supramolecular interactions, reappear in the title compound.

5. Synthesis and crystallization

The unsolvated compound (II) was prepared by addition of a solution of *n*-butyllithium (1.6 *M* in hexane, 1.5 ml, 2.3 mmol) to a cold solution (195 K) of 2,2′′-diiodo-1,1′:4′,1′′-terphenyl (0.5 g, 1.0 mmol) in 20 ml of dry THF. After 45 min of stirring, 4,4′-dichlorobenzophenone (0.52 g, 2.1 mmol), dissolved in 4 ml benzene and 15 ml THF, was added. The colourless reaction mixture was warmed to room temperature and stirred for 4 h. The solution was extracted twice with diethyl ether. The combined organic extracts were washed with water, dried over anhydrous sodium sulfate and concentrated under reduced pressure. Colourless crystals were isolated by recrystallization from hexane (yield: 7.0%). M.p. 543–546 K; ESI–MS $[M + H]^-$ *m*/*z* 731.3. IR (KBr) ν (cm^{-1}) 3547, 3056, 3025, 1913, 1641, 1591, 1575, 1489, 1331, 1182, 1157, 1097, 1014, 919, 903, 840, 761. ^{1}H NMR (500.1 MHz; $CDCl_3$): δ = 2.84 (2H, *s*, OH, 6.67 (4H, *s*, ArH), 6.75 (2H, *d*, $^3J_{HH}$ = 7.80 Hz, ArH), 7.09 (8H, *d*, $^3J_{HH}$ = 8.50 Hz, ArH), 7.11 (2H, *d*, $^3J_{HH}$ = 8.00 Hz, ArH), 7.22 (2H, *t*, $^3J_{HH}$ = 7.50 Hz, ArH), 7.26 (8H, *d*, $^3J_{HH}$ = 9.00 Hz, ArH), 7.32 (2H, *t*, $^3J_{HH}$ = 7.25 Hz, ArH). ^{13}C NMR (125.7 MHz, $CDCl_3$): δ = 82.68 (C-OH), 126.89, 127.43, 128.10, 129.11, 129.33, 129.83, 133.40, 140.24, 141.01, 144.06, 145.58 (Ar-C). EA calculated for $C_{44}H_{30}O_2Cl_4$: C 72.1, H 4.1%; found: C 72.2, H 4.4%. Crystals of (II*a*) suitable for X-ray diffraction were obtained from a solution of (II) in triethylamine upon slow evaporation of the solvent at room temperature.

6. Refinement details

Crystal data, data collection and structure refinement details are summarized in Table 2. All H atoms were placed geometrically in idealized positions and allowed to ride on their parent atoms, with C—H = 0.95 and 0.98 Å and U_{iso}(H) = 1.2U_{eq}(C) for aromatic and methylene, with C—H = 0.98 and O—H = 0.84 Å and U_{iso}(H) = 1.5U_{eq}(C) for methyl and hydroxy groups, respectively. Two molecules of triethylamine are each disordered over two positions with occupancy ratios of 0.567 (3):0.433 (3) and 0.503 (3):0.497 (3). They were modelled with restrained bond lengths based on average values of 1.47 (1) Å for N—C and 1.53 (1) Å for C—C bonds.

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supporting information

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Crystal structure of 2,2′′-bis(2,7-dichloro-9-hydroxy-9*H*-fluoren-9-yl)-1,1′:4′,1′′-terphenyl triethylamine trisolvate

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Computing details

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Sheldrick, 2008); data reduction: *SAINT* (Bruker, 2008); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2013* (Sheldrick, 2015); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

2,2′′-Bis(2,7-dichloro-9-hydroxy-9*H*-fluoren-9-yl)-1,1′:4′,1′′-terphenyl triethylamine trisolvate

Crystal data

$C_{44}H_{26}Cl_4O_2\cdot 3C_6H_{15}N$
M_r = 1032.01
Triclinic, $P\overline{1}$
a = 14.5995 (2) Å
b = 14.8094 (2) Å
c = 15.7705 (3) Å
α = 68.373 (1)°
β = 66.837 (1)°
γ = 67.558 (1)°
V = 2800.13 (8) Å^3
Z = 2
$F(000)$ = 1096
D_x = 1.224 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9853 reflections
θ = 2.4–31.3°
μ = 0.26 mm^{-1}
T = 100 K
Plate, colourless
0.42 × 0.40 × 0.23 mm

Data collection

Bruker CCD area detector diffractometer
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2008)
T_{min} = 0.900, T_{max} = 0.943
53831 measured reflections
14031 independent reflections
11477 reflections with $I > 2\sigma(I)$
R_{int} = 0.025
θ_{max} = 28.4°, θ_{min} = 1.5°
h = −19→19
k = −19→19
l = −21→21

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.113
S = 1.01
14031 reflections
773 parameters
24 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0538P)^2 + 1.6165P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.59 e Å^{-3}
$\Delta\rho_{min}$ = −0.59 e Å^{-3}

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Cl1	0.60638 (3)	0.02641 (3)	0.36155 (3)	0.02782 (9)	
Cl2	0.59812 (3)	0.31311 (3)	−0.33671 (3)	0.02962 (9)	
O1	0.78230 (7)	0.18376 (8)	−0.03539 (7)	0.0199 (2)	
H1	0.7514	0.2398	−0.0220	0.030*	
C1	0.63440 (10)	0.12716 (10)	0.08381 (9)	0.0163 (2)	
C2	0.65868 (10)	0.07862 (10)	0.16874 (10)	0.0188 (3)	
H2	0.7279	0.0419	0.1697	0.023*	
C3	0.57796 (11)	0.08549 (11)	0.25318 (10)	0.0199 (3)	
C4	0.47565 (10)	0.13766 (11)	0.25341 (10)	0.0207 (3)	
H4	0.4220	0.1398	0.3120	0.025*	
C5	0.45285 (10)	0.18656 (11)	0.16705 (10)	0.0198 (3)	
H5	0.3835	0.2226	0.1661	0.024*	
C6	0.53259 (10)	0.18211 (10)	0.08225 (10)	0.0171 (3)	
C7	0.53127 (10)	0.22501 (10)	−0.01767 (10)	0.0177 (3)	
C8	0.45058 (11)	0.28265 (11)	−0.05765 (11)	0.0225 (3)	
H8	0.3818	0.3026	−0.0180	0.027*	
C9	0.47169 (12)	0.31085 (11)	−0.15657 (11)	0.0250 (3)	
H9	0.4175	0.3500	−0.1851	0.030*	
C10	0.57288 (12)	0.28102 (11)	−0.21279 (10)	0.0221 (3)	
C11	0.65509 (11)	0.22404 (10)	−0.17454 (10)	0.0196 (3)	
H11	0.7240	0.2051	−0.2144	0.024*	
C12	0.63267 (10)	0.19620 (10)	−0.07658 (10)	0.0172 (3)	
C13	0.70829 (10)	0.13336 (10)	−0.01747 (9)	0.0163 (2)	
C14	0.76933 (10)	0.03037 (10)	−0.04016 (9)	0.0180 (3)	
C15	0.87711 (11)	0.00223 (11)	−0.06259 (10)	0.0220 (3)	
H15	0.9098	0.0451	−0.0596	0.026*	
C16	0.93772 (12)	−0.08693 (12)	−0.08910 (11)	0.0288 (3)	
H16	1.0111	−0.1043	−0.1046	0.035*	
C17	0.89114 (13)	−0.15025 (13)	−0.09285 (13)	0.0339 (4)	
H17	0.9321	−0.2113	−0.1111	0.041*	
C18	0.78417 (13)	−0.12403 (12)	−0.06975 (12)	0.0297 (3)	
H18	0.7526	−0.1680	−0.0724	0.036*	
C19	0.72127 (11)	−0.03479 (11)	−0.04260 (10)	0.0211 (3)	
C20	0.60696 (11)	−0.01430 (10)	−0.02017 (10)	0.0201 (3)	
C21	0.54278 (11)	−0.03021 (11)	0.07381 (10)	0.0212 (3)	
H21	0.5716	−0.0514	0.1249	0.025*	
C22	0.43748 (11)	−0.01550 (11)	0.09362 (10)	0.0216 (3)	
H22	0.3950	−0.0258	0.1580	0.026*	
Cl1A	0.92106 (3)	0.86051 (4)	0.13781 (3)	0.03593 (11)	

Cl2A	0.87208 (4)	0.64484 (3)	0.84734 (3)	0.04199 (12)
O1A	0.71671 (7)	0.87036 (7)	0.52729 (7)	0.01877 (19)
H1A	0.7474	0.9119	0.5195	0.028*
C1A	0.87109 (10)	0.78873 (10)	0.41745 (10)	0.0163 (2)
C2A	0.85448 (10)	0.81792 (10)	0.32984 (10)	0.0186 (3)
H2A	0.7870	0.8343	0.3246	0.022*
C3A	0.94014 (11)	0.82247 (11)	0.24930 (10)	0.0219 (3)
C4A	1.04014 (11)	0.79780 (11)	0.25515 (11)	0.0237 (3)
H4A	1.0974	0.7998	0.1989	0.028*
C5A	1.05506 (10)	0.77022 (11)	0.34418 (11)	0.0213 (3)
H5A	1.1225	0.7541	0.3494	0.026*
C6A	0.97026 (10)	0.76652 (10)	0.42527 (10)	0.0178 (3)
C7A	0.96262 (11)	0.73781 (10)	0.52698 (10)	0.0192 (3)
C8A	1.03705 (12)	0.71089 (11)	0.57298 (12)	0.0265 (3)
H8A	1.1068	0.7106	0.5373	0.032*
C9A	1.00714 (13)	0.68452 (12)	0.67219 (12)	0.0308 (4)
H9A	1.0565	0.6669	0.7049	0.037*
C10A	0.90563 (13)	0.68397 (12)	0.72328 (11)	0.0284 (3)
C11A	0.82964 (12)	0.71172 (11)	0.67874 (11)	0.0239 (3)
H11A	0.7600	0.7116	0.7147	0.029*
C12A	0.85985 (11)	0.73933 (10)	0.58041 (10)	0.0184 (3)
C13A	0.79079 (10)	0.77627 (10)	0.51543 (9)	0.0162 (2)
C14A	0.73042 (10)	0.70199 (10)	0.53606 (9)	0.0166 (2)
C15A	0.62299 (10)	0.73819 (11)	0.55279 (10)	0.0199 (3)
H15A	0.5905	0.8085	0.5461	0.024*
C16A	0.56284 (11)	0.67338 (12)	0.57902 (11)	0.0245 (3)
H16A	0.4899	0.6995	0.5902	0.029*
C17A	0.60905 (11)	0.57107 (12)	0.58886 (11)	0.0269 (3)
H17A	0.5681	0.5262	0.6082	0.032*
C18A	0.71616 (11)	0.53410 (11)	0.57025 (11)	0.0238 (3)
H18A	0.7478	0.4637	0.5765	0.029*
C19A	0.77833 (10)	0.59803 (10)	0.54256 (9)	0.0175 (3)
C20A	0.89299 (10)	0.55012 (10)	0.52056 (10)	0.0167 (2)
C21A	0.95553 (10)	0.55419 (10)	0.42644 (10)	0.0186 (3)
H21A	0.9256	0.5909	0.3756	0.022*
C22A	1.06098 (10)	0.50521 (10)	0.40625 (10)	0.0186 (3)
H22A	1.1023	0.5094	0.3417	0.022*
N1B	0.21028 (9)	0.98034 (9)	0.47727 (9)	0.0206 (2)
C1B	0.11268 (11)	0.96584 (13)	0.55043 (11)	0.0272 (3)
H1B1	0.0968	0.9098	0.5440	0.033*
H1B2	0.0559	1.0279	0.5385	0.033*
C2B	0.11490 (14)	0.94238 (14)	0.65192 (12)	0.0339 (4)
H2B1	0.1588	0.8735	0.6697	0.051*
H2B2	0.0443	0.9479	0.6955	0.051*
H2B3	0.1430	0.9905	0.6561	0.051*
C3B	0.19718 (12)	1.02007 (11)	0.38051 (11)	0.0238 (3)
H3B1	0.2584	1.0438	0.3357	0.029*
H3B2	0.1358	1.0798	0.3810	0.029*

C4B	0.18392 (13)	0.94741 (13)	0.34101 (12)	0.0294 (3)	
H4B1	0.2465	0.8903	0.3347	0.044*	
H4B2	0.1726	0.9829	0.2783	0.044*	
H4B3	0.1241	0.9224	0.3847	0.044*	
C5B	0.29651 (11)	0.88733 (11)	0.48674 (11)	0.0239 (3)	
H5B1	0.2804	0.8329	0.4777	0.029*	
H5B2	0.3021	0.8660	0.5523	0.029*	
C6B	0.40009 (12)	0.89960 (13)	0.41604 (12)	0.0298 (3)	
H6B1	0.3980	0.9125	0.3512	0.045*	
H6B2	0.4549	0.8376	0.4300	0.045*	
H6B3	0.4144	0.9566	0.4212	0.045*	
N1C	0.7405 (9)	0.5936 (6)	0.2422 (6)	0.0241 (7)	0.433 (3)
C1C	0.7208 (4)	0.5371 (4)	0.3433 (3)	0.0351 (10)	0.433 (3)
H1C1	0.6697	0.5835	0.3830	0.042*	0.433 (3)
H1C2	0.7860	0.5122	0.3607	0.042*	0.433 (3)
C2C	0.6805 (5)	0.4481 (6)	0.3656 (7)	0.0465 (19)	0.433 (3)
H2C1	0.6252	0.4693	0.3362	0.070*	0.433 (3)
H2C2	0.6531	0.4236	0.4349	0.070*	0.433 (3)
H2C3	0.7372	0.3937	0.3403	0.070*	0.433 (3)
C3C	0.7547 (3)	0.6915 (3)	0.2294 (3)	0.0287 (9)	0.433 (3)
H3C1	0.7755	0.7248	0.1603	0.034*	0.433 (3)
H3C2	0.8118	0.6794	0.2547	0.034*	0.433 (3)
C4C	0.6581 (11)	0.7621 (9)	0.2788 (9)	0.032 (2)	0.433 (3)
H4C1	0.5981	0.7635	0.2644	0.048*	0.433 (3)
H4C2	0.6667	0.8304	0.2560	0.048*	0.433 (3)
H4C3	0.6472	0.7382	0.3479	0.048*	0.433 (3)
C5C	0.8334 (3)	0.5338 (3)	0.1848 (3)	0.0249 (9)	0.433 (3)
H5C1	0.8277	0.4643	0.2023	0.030*	0.433 (3)
H5C2	0.8950	0.5294	0.1999	0.030*	0.433 (3)
C6C	0.8489 (12)	0.5789 (8)	0.0782 (6)	0.0329 (16)	0.433 (3)
H6C1	0.7852	0.5905	0.0638	0.049*	0.433 (3)
H6C2	0.9061	0.5319	0.0433	0.049*	0.433 (3)
H6C3	0.8653	0.6432	0.0587	0.049*	0.433 (3)
N1CA	0.7332 (7)	0.5984 (5)	0.2574 (5)	0.0241 (7)	0.567 (3)
C1CA	0.7446 (3)	0.4958 (3)	0.3206 (3)	0.0325 (8)	0.567 (3)
H1C3	0.7813	0.4879	0.3652	0.039*	0.567 (3)
H1C4	0.7883	0.4467	0.2816	0.039*	0.567 (3)
C2CA	0.6425 (4)	0.4705 (4)	0.3782 (5)	0.0396 (11)	0.567 (3)
H2C4	0.5999	0.5168	0.4192	0.059*	0.567 (3)
H2C5	0.6558	0.4008	0.4178	0.059*	0.567 (3)
H2C6	0.6059	0.4775	0.3347	0.059*	0.567 (3)
C3CA	0.6975 (2)	0.6728 (2)	0.3129 (2)	0.0286 (7)	0.567 (3)
H3C3	0.7560	0.6695	0.3319	0.034*	0.567 (3)
H3C4	0.6424	0.6543	0.3719	0.034*	0.567 (3)
C4CA	0.6558 (9)	0.7806 (7)	0.2589 (7)	0.0307 (17)	0.567 (3)
H4C4	0.7103	0.8000	0.2009	0.046*	0.567 (3)
H4C5	0.6338	0.8262	0.2995	0.046*	0.567 (3)
H4C6	0.5965	0.7850	0.2415	0.046*	0.567 (3)

C5CA	0.8318 (2)	0.6070 (3)	0.1833 (2)	0.0359 (8)	0.567 (3)
H5C3	0.8891	0.5724	0.2128	0.043*	0.567 (3)
H5C4	0.8303	0.6793	0.1563	0.043*	0.567 (3)
C6CA	0.8528 (10)	0.5612 (7)	0.1033 (5)	0.0468 (19)	0.567 (3)
H6C4	0.8599	0.4885	0.1289	0.070*	0.567 (3)
H6C5	0.9171	0.5720	0.0539	0.070*	0.567 (3)
H6C6	0.7951	0.5935	0.0755	0.070*	0.567 (3)
N1D	0.7016 (5)	0.3706 (6)	1.0068 (3)	0.0238 (9)	0.497 (3)
C1D	0.6422 (3)	0.4484 (3)	0.9448 (3)	0.0369 (9)	0.497 (3)
H1D1	0.6234	0.5137	0.9597	0.044*	0.497 (3)
H1D2	0.5770	0.4322	0.9592	0.044*	0.497 (3)
C2D	0.6979 (5)	0.4605 (4)	0.8397 (4)	0.0554 (14)	0.497 (3)
H2D1	0.7587	0.4838	0.8232	0.083*	0.497 (3)
H2D2	0.6510	0.5101	0.8029	0.083*	0.497 (3)
H2D3	0.7203	0.3953	0.8248	0.083*	0.497 (3)
C3D	0.6371 (4)	0.3527 (3)	1.1070 (3)	0.0395 (10)	0.497 (3)
H3D1	0.6761	0.2907	1.1443	0.047*	0.497 (3)
H3D2	0.5743	0.3391	1.1102	0.047*	0.497 (3)
C4D	0.6026 (4)	0.4366 (3)	1.1557 (3)	0.0509 (12)	0.497 (3)
H4D1	0.6630	0.4437	1.1628	0.076*	0.497 (3)
H4D2	0.5532	0.4200	1.2188	0.076*	0.497 (3)
H4D3	0.5692	0.5004	1.1169	0.076*	0.497 (3)
C5D	0.7959 (5)	0.3981 (8)	0.9893 (7)	0.056 (4)	0.497 (3)
H5D1	0.8162	0.3669	1.0490	0.067*	0.497 (3)
H5D2	0.7756	0.4722	0.9797	0.067*	0.497 (3)
C6D	0.8967 (2)	0.3713 (3)	0.9051 (3)	0.0386 (9)	0.497 (3)
H6D1	0.9136	0.3001	0.9067	0.058*	0.497 (3)
H6D2	0.9546	0.3831	0.9123	0.058*	0.497 (3)
H6D3	0.8845	0.4141	0.8440	0.058*	0.497 (3)
N1DA	0.7094 (5)	0.3795 (6)	0.9764 (3)	0.0238 (9)	0.503 (3)
C1DA	0.6889 (3)	0.4252 (3)	0.8834 (3)	0.0280 (8)	0.503 (3)
H1D3	0.6261	0.4101	0.8888	0.034*	0.503 (3)
H1D4	0.7475	0.3912	0.8365	0.034*	0.503 (3)
C2DA	0.6733 (3)	0.5392 (2)	0.8428 (3)	0.0366 (9)	0.503 (3)
H2D4	0.6176	0.5744	0.8892	0.055*	0.503 (3)
H2D5	0.6548	0.5611	0.7835	0.055*	0.503 (3)
H2D6	0.7377	0.5551	0.8296	0.055*	0.503 (3)
C3DA	0.6148 (3)	0.4082 (3)	1.0529 (3)	0.0336 (8)	0.503 (3)
H3D3	0.5569	0.3955	1.0455	0.040*	0.503 (3)
H3D4	0.5973	0.4817	1.0456	0.040*	0.503 (3)
C4DA	0.6240 (4)	0.3518 (4)	1.1529 (3)	0.0454 (11)	0.503 (3)
H4D4	0.6519	0.2791	1.1577	0.068*	0.503 (3)
H4D5	0.5554	0.3651	1.1996	0.068*	0.503 (3)
H4D6	0.6707	0.3748	1.1658	0.068*	0.503 (3)
C5DA	0.7983 (5)	0.3993 (5)	0.9831 (4)	0.025 (2)	0.503 (3)
H5D3	0.7715	0.4619	1.0048	0.030*	0.503 (3)
H5D4	0.8463	0.4135	0.9179	0.030*	0.503 (3)
C6DA	0.8645 (4)	0.3148 (4)	1.0504 (5)	0.085 (2)	0.503 (3)

H6D4	0.8256	0.3145	1.1172	0.127*	0.503 (3)
H6D5	0.9303	0.3293	1.0345	0.127*	0.503 (3)
H6D6	0.8784	0.2485	1.0408	0.127*	0.503 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.02612 (17)	0.0363 (2)	0.01956 (17)	−0.00544 (15)	−0.00797 (13)	−0.00754 (14)
Cl2	0.0435 (2)	0.02378 (18)	0.02120 (17)	−0.00960 (16)	−0.01303 (15)	−0.00132 (14)
O1	0.0167 (4)	0.0196 (5)	0.0260 (5)	−0.0077 (4)	−0.0024 (4)	−0.0100 (4)
C1	0.0167 (6)	0.0149 (6)	0.0184 (6)	−0.0050 (5)	−0.0030 (5)	−0.0072 (5)
C2	0.0169 (6)	0.0189 (7)	0.0210 (7)	−0.0038 (5)	−0.0049 (5)	−0.0077 (5)
C3	0.0224 (6)	0.0214 (7)	0.0175 (6)	−0.0059 (5)	−0.0064 (5)	−0.0061 (5)
C4	0.0188 (6)	0.0226 (7)	0.0197 (7)	−0.0045 (5)	−0.0018 (5)	−0.0098 (5)
C5	0.0164 (6)	0.0193 (7)	0.0231 (7)	−0.0027 (5)	−0.0042 (5)	−0.0088 (5)
C6	0.0179 (6)	0.0138 (6)	0.0209 (6)	−0.0041 (5)	−0.0058 (5)	−0.0061 (5)
C7	0.0192 (6)	0.0141 (6)	0.0215 (7)	−0.0053 (5)	−0.0060 (5)	−0.0056 (5)
C8	0.0214 (6)	0.0199 (7)	0.0259 (7)	−0.0036 (5)	−0.0085 (5)	−0.0061 (6)
C9	0.0285 (7)	0.0195 (7)	0.0281 (8)	−0.0039 (6)	−0.0144 (6)	−0.0036 (6)
C10	0.0331 (7)	0.0169 (7)	0.0187 (7)	−0.0096 (6)	−0.0100 (6)	−0.0017 (5)
C11	0.0239 (6)	0.0164 (6)	0.0195 (6)	−0.0085 (5)	−0.0045 (5)	−0.0047 (5)
C12	0.0201 (6)	0.0131 (6)	0.0209 (6)	−0.0064 (5)	−0.0064 (5)	−0.0048 (5)
C13	0.0160 (6)	0.0164 (6)	0.0175 (6)	−0.0058 (5)	−0.0034 (5)	−0.0057 (5)
C14	0.0200 (6)	0.0165 (6)	0.0152 (6)	−0.0047 (5)	−0.0028 (5)	−0.0047 (5)
C15	0.0210 (6)	0.0214 (7)	0.0208 (7)	−0.0051 (5)	−0.0039 (5)	−0.0056 (5)
C16	0.0228 (7)	0.0272 (8)	0.0287 (8)	−0.0016 (6)	−0.0022 (6)	−0.0102 (6)
C17	0.0333 (8)	0.0233 (8)	0.0383 (9)	0.0001 (6)	−0.0033 (7)	−0.0168 (7)
C18	0.0343 (8)	0.0215 (8)	0.0348 (9)	−0.0079 (6)	−0.0062 (7)	−0.0131 (6)
C19	0.0239 (7)	0.0176 (7)	0.0207 (7)	−0.0060 (5)	−0.0043 (5)	−0.0061 (5)
C20	0.0251 (7)	0.0140 (6)	0.0236 (7)	−0.0086 (5)	−0.0049 (5)	−0.0064 (5)
C21	0.0290 (7)	0.0180 (7)	0.0205 (7)	−0.0113 (6)	−0.0078 (5)	−0.0036 (5)
C22	0.0279 (7)	0.0198 (7)	0.0191 (7)	−0.0127 (6)	−0.0020 (5)	−0.0059 (5)
Cl1A	0.03125 (19)	0.0573 (3)	0.01955 (18)	−0.02149 (19)	−0.00780 (14)	−0.00025 (17)
Cl2A	0.0673 (3)	0.0322 (2)	0.0268 (2)	0.0014 (2)	−0.0264 (2)	−0.01023 (17)
O1A	0.0177 (4)	0.0138 (5)	0.0242 (5)	−0.0014 (4)	−0.0060 (4)	−0.0075 (4)
C1A	0.0158 (6)	0.0128 (6)	0.0202 (6)	−0.0029 (5)	−0.0052 (5)	−0.0055 (5)
C2A	0.0175 (6)	0.0183 (6)	0.0211 (7)	−0.0053 (5)	−0.0067 (5)	−0.0048 (5)
C3A	0.0238 (7)	0.0246 (7)	0.0182 (7)	−0.0100 (6)	−0.0067 (5)	−0.0026 (5)
C4A	0.0197 (6)	0.0255 (7)	0.0236 (7)	−0.0098 (6)	−0.0026 (5)	−0.0042 (6)
C5A	0.0167 (6)	0.0193 (7)	0.0291 (7)	−0.0060 (5)	−0.0076 (5)	−0.0055 (6)
C6A	0.0189 (6)	0.0130 (6)	0.0244 (7)	−0.0033 (5)	−0.0091 (5)	−0.0061 (5)
C7A	0.0224 (6)	0.0124 (6)	0.0262 (7)	−0.0022 (5)	−0.0123 (5)	−0.0058 (5)
C8A	0.0278 (7)	0.0204 (7)	0.0374 (9)	−0.0027 (6)	−0.0198 (6)	−0.0073 (6)
C9A	0.0416 (9)	0.0212 (7)	0.0394 (9)	0.0005 (6)	−0.0295 (8)	−0.0088 (7)
C10A	0.0446 (9)	0.0183 (7)	0.0250 (7)	0.0008 (6)	−0.0199 (7)	−0.0079 (6)
C11A	0.0312 (7)	0.0175 (7)	0.0231 (7)	0.0004 (6)	−0.0118 (6)	−0.0086 (6)
C12A	0.0232 (6)	0.0125 (6)	0.0221 (7)	−0.0007 (5)	−0.0106 (5)	−0.0073 (5)
C13A	0.0164 (6)	0.0142 (6)	0.0176 (6)	−0.0014 (5)	−0.0056 (5)	−0.0058 (5)

C14A	0.0180 (6)	0.0169 (6)	0.0138 (6)	−0.0047 (5)	−0.0038 (5)	−0.0040 (5)
C15A	0.0189 (6)	0.0185 (7)	0.0206 (7)	−0.0027 (5)	−0.0053 (5)	−0.0064 (5)
C16A	0.0176 (6)	0.0275 (8)	0.0260 (7)	−0.0066 (6)	−0.0041 (5)	−0.0064 (6)
C17A	0.0237 (7)	0.0242 (8)	0.0319 (8)	−0.0122 (6)	−0.0046 (6)	−0.0044 (6)
C18A	0.0238 (7)	0.0172 (7)	0.0281 (7)	−0.0067 (5)	−0.0059 (6)	−0.0041 (6)
C19A	0.0184 (6)	0.0175 (6)	0.0159 (6)	−0.0044 (5)	−0.0043 (5)	−0.0046 (5)
C20A	0.0180 (6)	0.0119 (6)	0.0201 (6)	−0.0032 (5)	−0.0047 (5)	−0.0061 (5)
C21A	0.0219 (6)	0.0147 (6)	0.0185 (6)	−0.0031 (5)	−0.0074 (5)	−0.0042 (5)
C22A	0.0214 (6)	0.0162 (6)	0.0161 (6)	−0.0045 (5)	−0.0033 (5)	−0.0049 (5)
N1B	0.0200 (5)	0.0185 (6)	0.0241 (6)	−0.0034 (4)	−0.0066 (5)	−0.0084 (5)
C1B	0.0227 (7)	0.0299 (8)	0.0300 (8)	−0.0084 (6)	−0.0037 (6)	−0.0122 (6)
C2B	0.0356 (8)	0.0369 (9)	0.0271 (8)	−0.0120 (7)	−0.0035 (7)	−0.0101 (7)
C3B	0.0253 (7)	0.0212 (7)	0.0257 (7)	−0.0033 (6)	−0.0096 (6)	−0.0079 (6)
C4B	0.0301 (8)	0.0315 (8)	0.0323 (8)	−0.0045 (6)	−0.0114 (6)	−0.0161 (7)
C5B	0.0242 (7)	0.0189 (7)	0.0280 (7)	−0.0022 (5)	−0.0090 (6)	−0.0078 (6)
C6B	0.0223 (7)	0.0279 (8)	0.0356 (9)	−0.0011 (6)	−0.0078 (6)	−0.0110 (7)
N1C	0.0219 (12)	0.0267 (8)	0.0237 (19)	−0.0050 (8)	−0.0074 (13)	−0.0075 (9)
C1C	0.035 (2)	0.038 (3)	0.026 (2)	−0.009 (2)	−0.0104 (18)	−0.0003 (19)
C2C	0.034 (4)	0.055 (5)	0.038 (3)	−0.019 (3)	−0.008 (3)	0.005 (3)
C3C	0.0278 (17)	0.031 (2)	0.032 (2)	−0.0087 (15)	−0.0125 (15)	−0.0090 (15)
C4C	0.032 (3)	0.035 (5)	0.036 (4)	−0.007 (3)	−0.014 (3)	−0.015 (4)
C5C	0.0206 (15)	0.029 (2)	0.0225 (19)	−0.0028 (13)	−0.0084 (13)	−0.0057 (14)
C6C	0.034 (3)	0.035 (3)	0.023 (4)	−0.004 (3)	−0.008 (3)	−0.007 (3)
N1CA	0.0219 (12)	0.0267 (8)	0.0237 (19)	−0.0050 (8)	−0.0074 (13)	−0.0075 (9)
C1CA	0.0298 (17)	0.0235 (18)	0.046 (2)	−0.0022 (13)	−0.0211 (15)	−0.0059 (14)
C2CA	0.041 (3)	0.034 (2)	0.041 (3)	−0.017 (2)	−0.011 (3)	−0.0003 (17)
C3CA	0.0290 (13)	0.0302 (16)	0.0298 (15)	−0.0045 (11)	−0.0131 (11)	−0.0103 (12)
C4CA	0.029 (2)	0.025 (3)	0.039 (4)	−0.0059 (17)	−0.015 (2)	−0.005 (2)
C5CA	0.0266 (14)	0.046 (2)	0.0378 (17)	−0.0115 (13)	−0.0037 (12)	−0.0185 (14)
C6CA	0.039 (3)	0.060 (5)	0.041 (5)	−0.013 (3)	−0.005 (4)	−0.021 (4)
N1D	0.0213 (10)	0.0215 (14)	0.030 (3)	−0.0069 (8)	−0.0059 (19)	−0.009 (2)
C1D	0.0354 (18)	0.0319 (19)	0.041 (2)	0.0001 (15)	−0.0150 (16)	−0.0126 (16)
C2D	0.083 (4)	0.046 (3)	0.040 (3)	−0.020 (3)	−0.021 (3)	−0.008 (2)
C3D	0.061 (3)	0.036 (2)	0.029 (2)	−0.028 (2)	−0.001 (2)	−0.014 (2)
C4D	0.075 (3)	0.048 (3)	0.038 (2)	−0.033 (2)	0.001 (2)	−0.0221 (18)
C5D	0.018 (4)	0.058 (6)	0.112 (7)	−0.004 (4)	−0.012 (4)	−0.060 (5)
C6D	0.0235 (15)	0.0343 (19)	0.060 (2)	−0.0085 (14)	−0.0069 (15)	−0.0190 (17)
N1DA	0.0213 (10)	0.0215 (14)	0.030 (3)	−0.0069 (8)	−0.0059 (19)	−0.009 (2)
C1DA	0.0350 (18)	0.0208 (18)	0.033 (2)	−0.0121 (14)	−0.0138 (18)	−0.0029 (16)
C2DA	0.049 (2)	0.0192 (17)	0.048 (2)	−0.0123 (14)	−0.0269 (17)	0.0003 (14)
C3DA	0.0309 (16)	0.0271 (18)	0.039 (2)	−0.0080 (14)	−0.0002 (14)	−0.0149 (17)
C4DA	0.061 (3)	0.045 (3)	0.028 (2)	−0.024 (2)	0.004 (2)	−0.016 (2)
C5DA	0.034 (5)	0.019 (3)	0.026 (2)	−0.013 (3)	−0.012 (2)	0.000 (2)
C6DA	0.072 (3)	0.054 (3)	0.165 (7)	0.014 (3)	−0.083 (4)	−0.047 (4)

Geometric parameters (Å, º)

Cl1—C3	1.7427 (14)	C3B—H3B1	0.9900
Cl2—C10	1.7502 (15)	C3B—H3B2	0.9900
O1—C13	1.4229 (15)	C4B—H4B1	0.9800
O1—H1	0.8400	C4B—H4B2	0.9800
C1—C2	1.3804 (19)	C4B—H4B3	0.9800
C1—C6	1.4009 (18)	C5B—C6B	1.516 (2)
C1—C13	1.5282 (18)	C5B—H5B1	0.9900
C2—C3	1.3951 (19)	C5B—H5B2	0.9900
C2—H2	0.9500	C6B—H6B1	0.9800
C3—C4	1.3945 (19)	C6B—H6B2	0.9800
C4—C5	1.391 (2)	C6B—H6B3	0.9800
C4—H4	0.9500	N1C—C5C	1.466 (8)
C5—C6	1.3893 (18)	N1C—C1C	1.471 (8)
C5—H5	0.9500	N1C—C3C	1.473 (8)
C6—C7	1.4709 (19)	C1C—C2C	1.515 (8)
C7—C8	1.3906 (19)	C1C—H1C1	0.9900
C7—C12	1.4017 (18)	C1C—H1C2	0.9900
C8—C9	1.394 (2)	C2C—H2C1	0.9800
C8—H8	0.9500	C2C—H2C2	0.9800
C9—C10	1.387 (2)	C2C—H2C3	0.9800
C9—H9	0.9500	C3C—C4C	1.516 (9)
C10—C11	1.392 (2)	C3C—H3C1	0.9900
C11—C12	1.3782 (19)	C3C—H3C2	0.9900
C11—H11	0.9500	C4C—H4C1	0.9800
C12—C13	1.5296 (18)	C4C—H4C2	0.9800
C13—C14	1.5369 (19)	C4C—H4C3	0.9800
C14—C15	1.3945 (19)	C5C—C6C	1.521 (7)
C14—C19	1.4109 (19)	C5C—H5C1	0.9900
C15—C16	1.388 (2)	C5C—H5C2	0.9900
C15—H15	0.9500	C6C—H6C1	0.9800
C16—C17	1.380 (2)	C6C—H6C2	0.9800
C16—H16	0.9500	C6C—H6C3	0.9800
C17—C18	1.384 (2)	N1CA—C1CA	1.467 (6)
C17—H17	0.9500	N1CA—C5CA	1.470 (7)
C18—C19	1.398 (2)	N1CA—C3CA	1.470 (6)
C18—H18	0.9500	C1CA—C2CA	1.516 (5)
C19—C20	1.4935 (19)	C1CA—H1C3	0.9900
C20—C21	1.396 (2)	C1CA—H1C4	0.9900
C20—C22^{i}	1.398 (2)	C2CA—H2C4	0.9800
C21—C22	1.387 (2)	C2CA—H2C5	0.9800
C21—H21	0.9500	C2CA—H2C6	0.9800
C22—C20^{i}	1.398 (2)	C3CA—C4CA	1.519 (7)
C22—H22	0.9500	C3CA—H3C3	0.9900
Cl1A—C3A	1.7383 (15)	C3CA—H3C4	0.9900
Cl2A—C10A	1.7408 (16)	C4CA—H4C4	0.9800
O1A—C13A	1.4243 (15)	C4CA—H4C5	0.9800

O1A—H1A	0.8400	C4CA—H4C6	0.9800
C1A—C2A	1.3777 (19)	C5CA—C6CA	1.522 (7)
C1A—C6A	1.4022 (17)	C5CA—H5C3	0.9900
C1A—C13A	1.5252 (18)	C5CA—H5C4	0.9900
C2A—C3A	1.3905 (19)	C6CA—H6C4	0.9800
C2A—H2A	0.9500	C6CA—H6C5	0.9800
C3A—C4A	1.395 (2)	C6CA—H6C6	0.9800
C4A—C5A	1.391 (2)	N1D—C1D	1.452 (6)
C4A—H4A	0.9500	N1D—C3D	1.472 (6)
C5A—C6A	1.3877 (19)	N1D—C5D	1.478 (7)
C5A—H5A	0.9500	C1D—C2D	1.508 (5)
C6A—C7A	1.4693 (19)	C1D—H1D1	0.9900
C7A—C8A	1.3937 (19)	C1D—H1D2	0.9900
C7A—C12A	1.3983 (19)	C2D—H2D1	0.9800
C8A—C9A	1.390 (2)	C2D—H2D2	0.9800
C8A—H8A	0.9500	C2D—H2D3	0.9800
C9A—C10A	1.382 (2)	C3D—C4D	1.520 (5)
C9A—H9A	0.9500	C3D—H3D1	0.9900
C10A—C11A	1.395 (2)	C3D—H3D2	0.9900
C11A—C12A	1.378 (2)	C4D—H4D1	0.9800
C11A—H11A	0.9500	C4D—H4D2	0.9800
C12A—C13A	1.5311 (18)	C4D—H4D3	0.9800
C13A—C14A	1.5308 (18)	C5D—C6D	1.579 (7)
C14A—C15A	1.3978 (18)	C5D—H5D1	0.9900
C14A—C19A	1.4100 (19)	C5D—H5D2	0.9900
C15A—C16A	1.389 (2)	C6D—H6D1	0.9800
C15A—H15A	0.9500	C6D—H6D2	0.9800
C16A—C17A	1.380 (2)	C6D—H6D3	0.9800
C16A—H16A	0.9500	N1DA—C1DA	1.469 (6)
C17A—C18A	1.391 (2)	N1DA—C3DA	1.471 (6)
C17A—H17A	0.9500	N1DA—C5DA	1.484 (7)
C18A—C19A	1.3964 (19)	C1DA—C2DA	1.529 (4)
C18A—H18A	0.9500	C1DA—H1D3	0.9900
C19A—C20A	1.4979 (18)	C1DA—H1D4	0.9900
C20A—C22A^{ii}	1.3956 (19)	C2DA—H2D4	0.9800
C20A—C21A	1.3966 (19)	C2DA—H2D5	0.9800
C21A—C22A	1.3891 (19)	C2DA—H2D6	0.9800
C21A—H21A	0.9500	C3DA—C4DA	1.521 (5)
C22A—C20A^{ii}	1.3956 (19)	C3DA—H3D3	0.9900
C22A—H22A	0.9500	C3DA—H3D4	0.9900
N1B—C1B	1.4714 (18)	C4DA—H4D4	0.9800
N1B—C5B	1.4754 (18)	C4DA—H4D5	0.9800
N1B—C3B	1.4809 (19)	C4DA—H4D6	0.9800
C1B—C2B	1.519 (2)	C5DA—C6DA	1.589 (7)
C1B—H1B1	0.9900	C5DA—H5D3	0.9900
C1B—H1B2	0.9900	C5DA—H5D4	0.9900
C2B—H2B1	0.9800	C6DA—H6D4	0.9800
C2B—H2B2	0.9800	C6DA—H6D5	0.9800

C2B—H2B3	0.9800	C6DA—H6D6	0.9800
C3B—C4B	1.527 (2)		

C13—O1—H1	109.5	N1B—C5B—H5B1	108.9
C2—C1—C6	121.32 (12)	C6B—C5B—H5B1	108.9
C2—C1—C13	127.78 (12)	N1B—C5B—H5B2	108.9
C6—C1—C13	110.87 (11)	C6B—C5B—H5B2	108.9
C1—C2—C3	117.59 (12)	H5B1—C5B—H5B2	107.7
C1—C2—H2	121.2	C5B—C6B—H6B1	109.5
C3—C2—H2	121.2	C5B—C6B—H6B2	109.5
C4—C3—C2	122.09 (13)	H6B1—C6B—H6B2	109.5
C4—C3—Cl1	119.22 (11)	C5B—C6B—H6B3	109.5
C2—C3—Cl1	118.69 (11)	H6B1—C6B—H6B3	109.5
C5—C4—C3	119.43 (12)	H6B2—C6B—H6B3	109.5
C5—C4—H4	120.3	C5C—N1C—C1C	109.4 (7)
C3—C4—H4	120.3	C5C—N1C—C3C	110.0 (7)
C6—C5—C4	119.23 (12)	C1C—N1C—C3C	110.4 (7)
C6—C5—H5	120.4	N1C—C1C—C2C	113.1 (7)
C4—C5—H5	120.4	N1C—C1C—H1C1	109.0
C5—C6—C1	120.30 (13)	C2C—C1C—H1C1	109.0
C5—C6—C7	130.96 (12)	N1C—C1C—H1C2	109.0
C1—C6—C7	108.71 (11)	C2C—C1C—H1C2	109.0
C8—C7—C12	120.11 (13)	H1C1—C1C—H1C2	107.8
C8—C7—C6	131.60 (13)	C1C—C2C—H2C1	109.5
C12—C7—C6	108.27 (12)	C1C—C2C—H2C2	109.5
C7—C8—C9	119.29 (13)	H2C1—C2C—H2C2	109.5
C7—C8—H8	120.4	C1C—C2C—H2C3	109.5
C9—C8—H8	120.4	H2C1—C2C—H2C3	109.5
C10—C9—C8	119.12 (13)	H2C2—C2C—H2C3	109.5
C10—C9—H9	120.4	N1C—C3C—C4C	113.3 (8)
C8—C9—H9	120.4	N1C—C3C—H3C1	108.9
C9—C10—C11	122.68 (13)	C4C—C3C—H3C1	108.9
C9—C10—Cl2	118.86 (11)	N1C—C3C—H3C2	108.9
C11—C10—Cl2	118.44 (11)	C4C—C3C—H3C2	108.9
C12—C11—C10	117.41 (13)	H3C1—C3C—H3C2	107.7
C12—C11—H11	121.3	C3C—C4C—H4C1	109.5
C10—C11—H11	121.3	C3C—C4C—H4C2	109.5
C11—C12—C7	121.39 (13)	H4C1—C4C—H4C2	109.5
C11—C12—C13	127.54 (12)	C3C—C4C—H4C3	109.5
C7—C12—C13	111.07 (12)	H4C1—C4C—H4C3	109.5
O1—C13—C1	111.11 (10)	H4C2—C4C—H4C3	109.5
O1—C13—C12	111.35 (11)	N1C—C5C—C6C	112.6 (7)
C1—C13—C12	101.02 (10)	N1C—C5C—H5C1	109.1
O1—C13—C14	107.02 (10)	C6C—C5C—H5C1	109.1
C1—C13—C14	114.40 (11)	N1C—C5C—H5C2	109.1
C12—C13—C14	111.99 (11)	C6C—C5C—H5C2	109.1
C15—C14—C19	118.90 (13)	H5C1—C5C—H5C2	107.8
C15—C14—C13	118.26 (12)	C5C—C6C—H6C1	109.5

C19—C14—C13	122.80 (12)	C5C—C6C—H6C2	109.5
C16—C15—C14	121.50 (14)	H6C1—C6C—H6C2	109.5
C16—C15—H15	119.2	C5C—C6C—H6C3	109.5
C14—C15—H15	119.2	H6C1—C6C—H6C3	109.5
C17—C16—C15	119.80 (14)	H6C2—C6C—H6C3	109.5
C17—C16—H16	120.1	C1CA—N1CA—C5CA	110.5 (6)
C15—C16—H16	120.1	C1CA—N1CA—C3CA	110.3 (5)
C16—C17—C18	119.45 (15)	C5CA—N1CA—C3CA	110.3 (5)
C16—C17—H17	120.3	N1CA—C1CA—C2CA	113.7 (5)
C18—C17—H17	120.3	N1CA—C1CA—H1C3	108.8
C17—C18—C19	121.92 (15)	C2CA—C1CA—H1C3	108.8
C17—C18—H18	119.0	N1CA—C1CA—H1C4	108.8
C19—C18—H18	119.0	C2CA—C1CA—H1C4	108.8
C18—C19—C14	118.42 (13)	H1C3—C1CA—H1C4	107.7
C18—C19—C20	117.00 (13)	C1CA—C2CA—H2C4	109.5
C14—C19—C20	124.57 (12)	C1CA—C2CA—H2C5	109.5
C21—C20—C22^{i}	118.20 (13)	H2C4—C2CA—H2C5	109.5
C21—C20—C19	121.51 (13)	C1CA—C2CA—H2C6	109.5
C22^{i}—C20—C19	120.16 (13)	H2C4—C2CA—H2C6	109.5
C22—C21—C20	120.84 (13)	H2C5—C2CA—H2C6	109.5
C22—C21—H21	119.6	N1CA—C3CA—C4CA	113.5 (6)
C20—C21—H21	119.6	N1CA—C3CA—H3C3	108.9
C21—C22—C20^{i}	120.95 (13)	C4CA—C3CA—H3C3	108.9
C21—C22—H22	119.5	N1CA—C3CA—H3C4	108.9
C20^{i}—C22—H22	119.5	C4CA—C3CA—H3C4	108.9
C13A—O1A—H1A	109.5	H3C3—C3CA—H3C4	107.7
C2A—C1A—C6A	121.37 (12)	C3CA—C4CA—H4C4	109.5
C2A—C1A—C13A	127.42 (11)	C3CA—C4CA—H4C5	109.5
C6A—C1A—C13A	111.20 (12)	H4C4—C4CA—H4C5	109.5
C1A—C2A—C3A	117.54 (12)	C3CA—C4CA—H4C6	109.5
C1A—C2A—H2A	121.2	H4C4—C4CA—H4C6	109.5
C3A—C2A—H2A	121.2	H4C5—C4CA—H4C6	109.5
C2A—C3A—C4A	122.28 (13)	N1CA—C5CA—C6CA	112.3 (6)
C2A—C3A—Cl1A	118.45 (11)	N1CA—C5CA—H5C3	109.1
C4A—C3A—Cl1A	119.26 (11)	C6CA—C5CA—H5C3	109.1
C5A—C4A—C3A	119.30 (13)	N1CA—C5CA—H5C4	109.1
C5A—C4A—H4A	120.4	C6CA—C5CA—H5C4	109.1
C3A—C4A—H4A	120.4	H5C3—C5CA—H5C4	107.9
C6A—C5A—C4A	119.19 (12)	C5CA—C6CA—H6C4	109.5
C6A—C5A—H5A	120.4	C5CA—C6CA—H6C5	109.5
C4A—C5A—H5A	120.4	H6C4—C6CA—H6C5	109.5
C5A—C6A—C1A	120.27 (13)	C5CA—C6CA—H6C6	109.5
C5A—C6A—C7A	131.30 (12)	H6C4—C6CA—H6C6	109.5
C1A—C6A—C7A	108.37 (12)	H6C5—C6CA—H6C6	109.5
C8A—C7A—C12A	120.06 (14)	C1D—N1D—C3D	111.1 (5)
C8A—C7A—C6A	131.51 (14)	C1D—N1D—C5D	108.6 (6)
C12A—C7A—C6A	108.43 (11)	C3D—N1D—C5D	114.6 (5)
C9A—C8A—C7A	118.70 (15)	N1D—C1D—C2D	114.4 (4)

C9A—C8A—H8A	120.7	N1D—C1D—H1D1	108.7
C7A—C8A—H8A	120.7	C2D—C1D—H1D1	108.7
C10A—C9A—C8A	120.05 (14)	N1D—C1D—H1D2	108.7
C10A—C9A—H9A	120.0	C2D—C1D—H1D2	108.7
C8A—C9A—H9A	120.0	H1D1—C1D—H1D2	107.6
C9A—C10A—C11A	122.21 (15)	C1D—C2D—H2D1	109.5
C9A—C10A—Cl2A	118.90 (12)	C1D—C2D—H2D2	109.5
C11A—C10A—Cl2A	118.87 (13)	H2D1—C2D—H2D2	109.5
C12A—C11A—C10A	117.19 (15)	C1D—C2D—H2D3	109.5
C12A—C11A—H11A	121.4	H2D1—C2D—H2D3	109.5
C10A—C11A—H11A	121.4	H2D2—C2D—H2D3	109.5
C11A—C12A—C7A	121.76 (13)	N1D—C3D—C4D	117.0 (5)
C11A—C12A—C13A	127.11 (13)	N1D—C3D—H3D1	108.1
C7A—C12A—C13A	111.13 (12)	C4D—C3D—H3D1	108.1
O1A—C13A—C1A	111.32 (10)	N1D—C3D—H3D2	108.1
O1A—C13A—C14A	107.22 (10)	C4D—C3D—H3D2	108.1
C1A—C13A—C14A	114.25 (11)	H3D1—C3D—H3D2	107.3
O1A—C13A—C12A	110.73 (10)	C3D—C4D—H4D1	109.5
C1A—C13A—C12A	100.74 (10)	C3D—C4D—H4D2	109.5
C14A—C13A—C12A	112.58 (11)	H4D1—C4D—H4D2	109.5
C15A—C14A—C19A	118.83 (12)	C3D—C4D—H4D3	109.5
C15A—C14A—C13A	118.53 (12)	H4D1—C4D—H4D3	109.5
C19A—C14A—C13A	122.59 (11)	H4D2—C4D—H4D3	109.5
C16A—C15A—C14A	121.32 (13)	N1D—C5D—C6D	121.3 (7)
C16A—C15A—H15A	119.3	N1D—C5D—H5D1	107.0
C14A—C15A—H15A	119.3	C6D—C5D—H5D1	107.0
C17A—C16A—C15A	119.96 (13)	N1D—C5D—H5D2	107.0
C17A—C16A—H16A	120.0	C6D—C5D—H5D2	107.0
C15A—C16A—H16A	120.0	H5D1—C5D—H5D2	106.7
C16A—C17A—C18A	119.45 (13)	C5D—C6D—H6D1	109.5
C16A—C17A—H17A	120.3	C5D—C6D—H6D2	109.5
C18A—C17A—H17A	120.3	H6D1—C6D—H6D2	109.5
C17A—C18A—C19A	121.57 (14)	C5D—C6D—H6D3	109.5
C17A—C18A—H18A	119.2	H6D1—C6D—H6D3	109.5
C19A—C18A—H18A	119.2	H6D2—C6D—H6D3	109.5
C18A—C19A—C14A	118.79 (12)	C1DA—N1DA—C3DA	110.3 (5)
C18A—C19A—C20A	116.71 (12)	C1DA—N1DA—C5DA	115.5 (5)
C14A—C19A—C20A	124.50 (12)	C3DA—N1DA—C5DA	110.9 (5)
C22A^{ii}—C20A—C21A	118.27 (12)	N1DA—C1DA—C2DA	117.3 (4)
C22A^{ii}—C20A—C19A	120.83 (12)	N1DA—C1DA—H1D3	108.0
C21A—C20A—C19A	120.78 (12)	C2DA—C1DA—H1D3	108.0
C22A—C21A—C20A	120.81 (13)	N1DA—C1DA—H1D4	108.0
C22A—C21A—H21A	119.6	C2DA—C1DA—H1D4	108.0
C20A—C21A—H21A	119.6	H1D3—C1DA—H1D4	107.2
C21A—C22A—C20A^{ii}	120.92 (12)	C1DA—C2DA—H2D4	109.5
C21A—C22A—H22A	119.5	C1DA—C2DA—H2D5	109.5
C20A^{ii}—C22A—H22A	119.5	H2D4—C2DA—H2D5	109.5
C1B—N1B—C5B	111.33 (12)	C1DA—C2DA—H2D6	109.5

C1B—N1B—C3B	110.96 (11)	H2D4—C2DA—H2D6	109.5
C5B—N1B—C3B	113.05 (11)	H2D5—C2DA—H2D6	109.5
N1B—C1B—C2B	113.88 (13)	N1DA—C3DA—C4DA	113.9 (4)
N1B—C1B—H1B1	108.8	N1DA—C3DA—H3D3	108.8
C2B—C1B—H1B1	108.8	C4DA—C3DA—H3D3	108.8
N1B—C1B—H1B2	108.8	N1DA—C3DA—H3D4	108.8
C2B—C1B—H1B2	108.8	C4DA—C3DA—H3D4	108.8
H1B1—C1B—H1B2	107.7	H3D3—C3DA—H3D4	107.7
C1B—C2B—H2B1	109.5	C3DA—C4DA—H4D4	109.5
C1B—C2B—H2B2	109.5	C3DA—C4DA—H4D5	109.5
H2B1—C2B—H2B2	109.5	H4D4—C4DA—H4D5	109.5
C1B—C2B—H2B3	109.5	C3DA—C4DA—H4D6	109.5
H2B1—C2B—H2B3	109.5	H4D4—C4DA—H4D6	109.5
H2B2—C2B—H2B3	109.5	H4D5—C4DA—H4D6	109.5
N1B—C3B—C4B	116.88 (13)	N1DA—C5DA—C6DA	118.7 (5)
N1B—C3B—H3B1	108.1	N1DA—C5DA—H5D3	107.6
C4B—C3B—H3B1	108.1	C6DA—C5DA—H5D3	107.6
N1B—C3B—H3B2	108.1	N1DA—C5DA—H5D4	107.6
C4B—C3B—H3B2	108.1	C6DA—C5DA—H5D4	107.6
H3B1—C3B—H3B2	107.3	H5D3—C5DA—H5D4	107.1
C3B—C4B—H4B1	109.5	C5DA—C6DA—H6D4	109.5
C3B—C4B—H4B2	109.5	C5DA—C6DA—H6D5	109.5
H4B1—C4B—H4B2	109.5	H6D4—C6DA—H6D5	109.5
C3B—C4B—H4B3	109.5	C5DA—C6DA—H6D6	109.5
H4B1—C4B—H4B3	109.5	H6D4—C6DA—H6D6	109.5
H4B2—C4B—H4B3	109.5	H6D5—C6DA—H6D6	109.5
N1B—C5B—C6B	113.51 (12)		

C6—C1—C2—C3	0.5 (2)	C5A—C6A—C7A—C12A	−175.28 (14)
C13—C1—C2—C3	178.35 (13)	C1A—C6A—C7A—C12A	2.01 (15)
C1—C2—C3—C4	1.1 (2)	C12A—C7A—C8A—C9A	0.9 (2)
C1—C2—C3—Cl1	−179.17 (10)	C6A—C7A—C8A—C9A	−178.38 (14)
C2—C3—C4—C5	−1.4 (2)	C7A—C8A—C9A—C10A	0.9 (2)
Cl1—C3—C4—C5	178.80 (11)	C8A—C9A—C10A—C11A	−1.7 (2)
C3—C4—C5—C6	0.2 (2)	C8A—C9A—C10A—Cl2A	176.99 (12)
C4—C5—C6—C1	1.4 (2)	C9A—C10A—C11A—C12A	0.6 (2)
C4—C5—C6—C7	179.40 (13)	Cl2A—C10A—C11A—C12A	−178.09 (11)
C2—C1—C6—C5	−1.8 (2)	C10A—C11A—C12A—C7A	1.3 (2)
C13—C1—C6—C5	−179.92 (12)	C10A—C11A—C12A—C13A	−177.59 (13)
C2—C1—C6—C7	179.81 (12)	C8A—C7A—C12A—C11A	−2.0 (2)
C13—C1—C6—C7	1.66 (15)	C6A—C7A—C12A—C11A	177.39 (12)
C5—C6—C7—C8	0.0 (3)	C8A—C7A—C12A—C13A	177.00 (12)
C1—C6—C7—C8	178.18 (14)	C6A—C7A—C12A—C13A	−3.57 (15)
C5—C6—C7—C12	−178.43 (14)	C2A—C1A—C13A—O1A	−64.61 (17)
C1—C6—C7—C12	−0.24 (15)	C6A—C1A—C13A—O1A	115.17 (12)
C12—C7—C8—C9	0.3 (2)	C2A—C1A—C13A—C14A	57.01 (18)
C6—C7—C8—C9	−177.96 (14)	C6A—C1A—C13A—C14A	−123.21 (12)
C7—C8—C9—C10	−0.3 (2)	C2A—C1A—C13A—C12A	177.95 (13)

C8—C9—C10—C11	−0.3 (2)
C8—C9—C10—Cl2	177.89 (11)
C9—C10—C11—C12	0.7 (2)
Cl2—C10—C11—C12	−177.43 (10)
C10—C11—C12—C7	−0.7 (2)
C10—C11—C12—C13	179.42 (12)
C8—C7—C12—C11	0.2 (2)
C6—C7—C12—C11	178.82 (12)
C8—C7—C12—C13	−179.90 (12)
C6—C7—C12—C13	−1.27 (15)
C2—C1—C13—O1	−62.04 (17)
C6—C1—C13—O1	115.96 (12)
C2—C1—C13—C12	179.74 (13)
C6—C1—C13—C12	−2.26 (14)
C2—C1—C13—C14	59.26 (18)
C6—C1—C13—C14	−122.74 (12)
C11—C12—C13—O1	63.97 (17)
C7—C12—C13—O1	−115.93 (12)
C11—C12—C13—C1	−177.99 (13)
C7—C12—C13—C1	2.11 (14)
C11—C12—C13—C14	−55.82 (17)
C7—C12—C13—C14	124.28 (12)
O1—C13—C14—C15	6.18 (16)
C1—C13—C14—C15	−117.35 (13)
C12—C13—C14—C15	128.47 (13)
O1—C13—C14—C19	−171.45 (12)
C1—C13—C14—C19	65.02 (17)
C12—C13—C14—C19	−49.16 (17)
C19—C14—C15—C16	1.4 (2)
C13—C14—C15—C16	−176.30 (13)
C14—C15—C16—C17	−0.6 (2)
C15—C16—C17—C18	−0.2 (3)
C16—C17—C18—C19	0.1 (3)
C17—C18—C19—C14	0.8 (2)
C17—C18—C19—C20	179.49 (15)
C15—C14—C19—C18	−1.5 (2)
C13—C14—C19—C18	176.09 (13)
C15—C14—C19—C20	179.91 (13)
C13—C14—C19—C20	−2.5 (2)
C18—C19—C20—C21	102.54 (17)
C14—C19—C20—C21	−78.87 (19)
C18—C19—C20—C22^{i}	−73.40 (18)
C14—C19—C20—C22^{i}	105.19 (17)
C22^{i}—C20—C21—C22	−0.8 (2)
C19—C20—C21—C22	−176.85 (13)
C20—C21—C22—C20^{i}	0.9 (2)
C6A—C1A—C2A—C3A	1.4 (2)
C13A—C1A—C2A—C3A	−178.87 (13)
C6A—C1A—C13A—C12A	−2.27 (14)
C11A—C12A—C13A—O1A	64.65 (17)
C7A—C12A—C13A—O1A	−114.32 (12)
C11A—C12A—C13A—C1A	−177.48 (13)
C7A—C12A—C13A—C1A	3.54 (14)
C11A—C12A—C13A—C14A	−55.37 (18)
C7A—C12A—C13A—C14A	125.66 (12)
O1A—C13A—C14A—C15A	5.45 (16)
C1A—C13A—C14A—C15A	−118.40 (13)
C12A—C13A—C14A—C15A	127.48 (13)
O1A—C13A—C14A—C19A	−171.97 (12)
C1A—C13A—C14A—C19A	64.18 (16)
C12A—C13A—C14A—C19A	−49.94 (17)
C19A—C14A—C15A—C16A	2.5 (2)
C13A—C14A—C15A—C16A	−175.04 (13)
C14A—C15A—C16A—C17A	−0.1 (2)
C15A—C16A—C17A—C18A	−1.4 (2)
C16A—C17A—C18A—C19A	0.6 (2)
C17A—C18A—C19A—C14A	1.8 (2)
C17A—C18A—C19A—C20A	−177.53 (14)
C15A—C14A—C19A—C18A	−3.2 (2)
C13A—C14A—C19A—C18A	174.17 (13)
C15A—C14A—C19A—C20A	176.00 (13)
C13A—C14A—C19A—C20A	−6.6 (2)
C18A—C19A—C20A—C22A^{ii}	−77.30 (17)
C14A—C19A—C20A—C22A^{ii}	103.44 (16)
C18A—C19A—C20A—C21A	98.52 (16)
C14A—C19A—C20A—C21A	−80.73 (18)
C22A^{ii}—C20A—C21A—C22A	−0.6 (2)
C19A—C20A—C21A—C22A	−176.54 (13)
C20A—C21A—C22A—C20A^{ii}	0.6 (2)
C5B—N1B—C1B—C2B	62.98 (17)
C3B—N1B—C1B—C2B	−170.17 (13)
C1B—N1B—C3B—C4B	−71.11 (16)
C5B—N1B—C3B—C4B	54.78 (17)
C1B—N1B—C5B—C6B	−177.19 (13)
C3B—N1B—C5B—C6B	57.12 (16)
C5C—N1C—C1C—C2C	−72.5 (10)
C3C—N1C—C1C—C2C	166.3 (7)
C5C—N1C—C3C—C4C	174.3 (9)
C1C—N1C—C3C—C4C	−64.8 (11)
C1C—N1C—C5C—C6C	170.4 (8)
C3C—N1C—C5C—C6C	−68.2 (11)
C5CA—N1CA—C1CA—C2CA	−161.8 (5)
C3CA—N1CA—C1CA—C2CA	75.9 (8)
C1CA—N1CA—C3CA—C4CA	−164.3 (7)
C5CA—N1CA—C3CA—C4CA	73.4 (9)
C1CA—N1CA—C5CA—C6CA	78.2 (8)

C1A—C2A—C3A—C4A	0.6 (2)	C3CA—N1CA—C5CA—C6CA	−159.6 (6)
C1A—C2A—C3A—Cl1A	−179.27 (11)	C3D—N1D—C1D—C2D	−171.4 (5)
C2A—C3A—C4A—C5A	−1.8 (2)	C5D—N1D—C1D—C2D	61.8 (7)
Cl1A—C3A—C4A—C5A	178.12 (11)	C1D—N1D—C3D—C4D	−69.0 (7)
C3A—C4A—C5A—C6A	0.9 (2)	C5D—N1D—C3D—C4D	54.4 (8)
C4A—C5A—C6A—C1A	1.0 (2)	C1D—N1D—C5D—C6D	−84.2 (9)
C4A—C5A—C6A—C7A	178.05 (14)	C3D—N1D—C5D—C6D	151.0 (7)
C2A—C1A—C6A—C5A	−2.2 (2)	C3DA—N1DA—C1DA—C2DA	72.0 (6)
C13A—C1A—C6A—C5A	177.97 (12)	C5DA—N1DA—C1DA—C2DA	−54.7 (7)
C2A—C1A—C6A—C7A	−179.86 (12)	C1DA—N1DA—C3DA—C4DA	171.1 (4)
C13A—C1A—C6A—C7A	0.34 (15)	C5DA—N1DA—C3DA—C4DA	−59.7 (6)
C5A—C6A—C7A—C8A	4.1 (3)	C1DA—N1DA—C5DA—C6DA	−147.3 (6)
C1A—C6A—C7A—C8A	−178.65 (15)	C3DA—N1DA—C5DA—C6DA	86.3 (8)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1*D*^{iii}	0.84	1.95	2.781 (2)	171
O1—H1···N1*DA*^{iii}	0.84	1.91	2.731 (2)	164
O1*A*—H1*A*···N1*B*^{iv}	0.84	1.94	2.766 (2)	167
C4—H4···O1*A*^{v}	0.95	2.54	3.489 (2)	175
C4*A*—H4*A*···O1^{vi}	0.95	2.47	3.403 (2)	168
C9—H9···N1*C*^{vii}	0.95	2.54	3.459 (2)	163
C9—H9···N1*CA*^{vii}	0.95	2.60	3.519 (2)	162
C2*DA*—H2*D*6···Cl2*A*	0.98	2.90	3.819 (4)	157
C15—H15···O1	0.95	2.22	2.621 (2)	104
C15*A*—H15*A*···O1*A*	0.95	2.23	2.626 (2)	104

Symmetry codes: (iii) *x*, *y*, *z*−1; (iv) −*x*+1, −*y*+2, −*z*+1; (v) −*x*+1, −*y*+1, −*z*+1; (vi) −*x*+2, −*y*+1, −*z*; (vii) −*x*+1, −*y*+1, −*z*.