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Triprolidinium dichloranilate–chloranilic acid–methanol–water (2/1/2/2)

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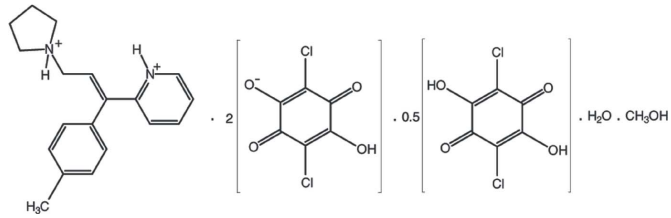
Key indicators: single-crystal X-ray study; T = 123 K; mean σ(C–C) = 0.004 Å; disorder in solvent or counterion; R factor = 0.052; wR factor = 0.137; data-to-parameter ratio = 14.8.

In the triprolidinium cation of the title compound {systematic name: 2-[1-(4-methylphenyl)-3-(pyrrolidin-1-ium-1-yl)prop-1-en-1-yl]pyridin-1-ium bis(2,5-dichloro-4-hydroxy-3,6-dioxocyclohexa-1,4-dien-1-olate)–2,5-dichloro-3,6-dihydroxycyclohexa-2,5-diene-1,4-dione–methanol–water (2/1/2/2)}, $C_{19}H_{24}N_2^{2+}\cdot 2C_6HCl_2O_4^-\cdot 0.5C_6H_2Cl_2O_4\cdot CH_3OH\cdot H_2O$, the N atoms on both the pyrrolidine and pyridine groups are protonated. The neutral chloranilic acid molecule is on an inversion symmetry element and its hydroxy H atoms are disordered over two positions with site-occupancy factors of 0.53 (6) and 0.47 (6). The methanol solvent molecule is disordered over two positions in a 0.836 (4):0.164 (4) ratio. In the crystal, N—H···O, O—H···O and C—H···O interactions link the components. The crystal structure also features π–π interactions between the benzene rings [centroid–centroid distances = 3.5674 (15), 3.5225 (15) and 3.6347 (15) Å].

Related literature

For the synthesis and spectroscopic studies of charge-transfer complexes between chloranilic acid and some heterocyclic amines in ethanol, see: Al-Attas *et al.* (2009). For spectroscopic studies of the interaction between triprolidine hydrochloride and serum albumins, see: Sandhya *et al.* (2011). For related structures, see: Adam *et al.* (2010); Dayananda *et al.* (2011); Dutkiewicz *et al.* (2010); Gotoh *et al.* (2010); Hakim Al-arique *et al.* (2010); Jasinski *et al.* (2010); Parvez & Sabir (1997); Udachin *et al.* (2011). For ring puckering parameters, see: Cremer & Pople (1975).



Experimental

Crystal data

$C_{19}H_{24}N_2^{2+}\cdot 2C_6HCl_2O_4^-\cdot 0.5C_6H_2Cl_2O_4\cdot CH_4O\cdot H_2O$
M_r = 850.88
Monoclinic, $P2_1/n$
a = 9.1633 (2) Å
b = 32.3720 (7) Å
c = 12.9834 (4) Å
β = 106.685 (3)°
V = 3689.17 (17) Å^3
Z = 4
Cu $K\alpha$ radiation
μ = 4.16 mm^{-1}
T = 123 K
0.5 × 0.38 × 0.12 mm

Data collection

Agilent Xcalibur Ruby Gemini diffractometer
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2011)
T_{min} = 0.188, T_{max} = 0.607
25133 measured reflections
7532 independent reflections
6721 reflections with $I > 2\sigma(I)$
R_{int} = 0.036

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.137
S = 1.08
7532 reflections
510 parameters
4 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 1.08 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O4A—H4AA···O3A	0.84	2.15	2.629 (3)	116
O4A—H4AA···O1W^{i}	0.84	1.92	2.672 (3)	148
N1—H1C···O3A	0.93	1.78	2.699 (3)	167
O2B—H2BA···O1B	0.84	2.19	2.655 (3)	115
O2B—H2BA···O1A^{ii}	0.84	2.50	3.012 (3)	121
O2B—H2BA···O2A^{ii}	0.84	2.08	2.776 (3)	139
N2—H2C···O3B	0.88	2.55	2.900 (3)	104
N2—H2C···O4B	0.88	1.79	2.667 (3)	175
O2C—H2CA···O1C^{iii}	0.84	2.21	2.680 (4)	116
O1W—H1$W1$···O1S	0.90 (3)	2.06 (3)	2.882 (3)	152 (4)
O1W—H1$W2$···O2B	0.82 (5)	2.18 (4)	2.976 (3)	162 (4)
C1—H1B···O1A^{iv}	0.99	2.34	3.286 (5)	160
C3—H3A···O1B^{v}	0.99	2.47	3.138 (5)	124
C4—H4B···O2A^{vi}	0.99	2.37	3.229 (3)	144
C4—H4B···O1B^{v}	0.99	2.34	2.994 (3)	123
C5—H5B···O1B^{v}	0.99	2.44	3.186 (3)	132
C9—H9A···Cl2A^{vi}	0.95	2.82	3.525 (3)	131
C9—H9A···O2A^{vi}	0.95	2.46	3.363 (3)	158
C18—H18A···Cl2B^{i}	0.95	2.68	3.467 (3)	140
C19—H19B···O1A^{ii}	0.98	2.55	3.102 (4)	116

Symmetry codes: (i) $x+\frac{1}{2}, -y+\frac{1}{2}, z-\frac{1}{2}$; (ii) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$; (iii) $-x+1, -y, -z+2$; (iv) $-x+2, -y+1, -z$; (v) $x-\frac{1}{2}, -y+\frac{1}{2}, z-\frac{1}{2}$; (vi) $-x+1, -y+1, -z$.

Data collection: *CrysAlis PRO* (Agilent, 2011); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis RED* (Agilent, 2011); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008);

molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5841).

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supporting information

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S1. Comment

Triprolidine (Systematic name: 2-[(*E*)-1-(4-methylphenyl)-3-pyrrolidin-1-yl-prop- 1-enyl]pyridine) is an over-the-counter antihistamine with anticholinergic properties. It is used to combat the symptoms associated with allergies and is sometimes combined with other cold medications designed to provide general relief for flu-like symptoms. Like many over-the-counter antihistamines, the most common side effect is drowsiness. Triprolidine is a quick acting drug that can clear congestion and stop runny noses in 15–30 minutes. The interaction between triprolidine hydrochloride (TRP) and serum albumins *viz*. bovine serum albumin (BSA) and human serum albumin (HSA) has been studied by spectroscopic methods (Sandhya *et al.*, 2011).

Chloranilic acid is a strong dibasic organic acid which exhibits electron-acceptor properties on one hand and acidic properties leading to formation of hydrogen bonds on the other hand. In the case of stronger bases the proton-transfer, hydrogen bonded ion pairs will be formed which is interesting from the point of view of electron transfer reactions in biological systems. Also, protonation of the donor from acidic acceptors are generally a route for the formation of ion pair adducts. The synthesis and spectroscopic studies of charge transfer complexes between chloranilic acid and some heterocyclic amines in ethanol (Al-Attas, Habeeb & Al-Raimi, 2009) have been studied. The crystal structures of triprolidine tetrachlorocuprate (II) (Parvez & Sabir, 1997), triethylammonium hydrogen chloranilate (Gotoh *et al.*, 2010), chloranilic acid: a redetermination at 100 K (Dutkiewicz *et al.*, 2010), bis(3-picoline) chloranilate chloranilic acid (Adam *et al.*, 2010), Gabapentin-lactum-chloranilic acid (Jasinski *et al.*, 2010), bis(2-{[3-methyl-4-(2,2,2-trifluoroethoxy)-2-pyridyl]methylsulfanyl}-1H,3*H*-benzimidazolium) 2,5-dichloro-3,6-dioxocyclohexa-1,4-diene-1,4-diolate (Hakim Al-arique *et al.*, 2010), bis(guanidinium) chloranilate (Udachin *et al.*, 2011) and triprolinidium dipicrate (Dayananda *et al.*, 2011) have been reported. In view of the importance of triprolidine, the paper reports the crystal structure of the title compound, (I).

As shown in Fig. 1, in the triprolidinium cation of (I), the N atoms on the pyridinium and pyrrolidine groups are protonated. The pyrrolidine group has an envelope conformation [the puckering parameters (Cremer & Pople, 1975) are Q(2) = 0.378 (4) Å, φ(2) = 1252.8 (5)°].

The crystal structure is stabilized by N—H···O, O—H···O and C—H···O interactions (Table 1, Fig. 2). Furthermore, the crystal structure is stabilized *via* π-π interactions between the benzene rings [*Cg*3···*Cg*5(*x*, *y*, *z*) = 3.5674 (15) Å, *Cg*3···*Cg*5(-1/2 + *x*, 1/2 - *y*, -1/2 + *z*) = 3.5225 (15) Å, *Cg*4···*Cg*4(2 - *x*, 1 - *y*, -*z*) = 3.6347 (15) Å; where *Cg*3, *Cg*4 and g5 are the centroids of the C13—C18, C1A–C6A and C1B–C6B benzene rings, respectively].

S2. Experimental

Triprolidine hydrochloride (3.148 g, 0.01 mol) in 10 ml of methanol was mixed with chloranilic acid (2.09 g, 0.01 mol) in 10 ml of methanol. The mixture was kept aside for three days at room temperature. The formed salt was filtered and dried in a vacuum desiccator over phosphorous pentoxide. The compound was recrystallized from methanol solution by slow

evaporation (m.p.: 448–450 K with charring).

S3. Refinement

The atoms of the methanol solvent molecule are disordered over two positions with the site-occupancy factors of 0.836 (4) and 0.164 (4). The hydroxyl H atoms of the neutral chloranilate molecule lying on an inversion centre are disordered over two positions with the site-occupancy factors of 0.53 (6) and 0.47 (6). The water H atoms were located in a difference Fourier map and refined with U_{iso}(H) = 1.5U_{eq}(O) and using the *DFIX* restraints for the O—H bond of 0.82 Å and the H···H distance of 1.297 Å. All of the remaining H atoms were placed in their calculated positions and refined using the riding model with C–H lengths of 0.84 Å (OH), 0.88 Å (NH), 0.93 Å (NH), 0.95 Å (CH), 0.99 Å (CH_2) or 0.98 Å (CH_3). Their isotropic displacement parameters were set to 1.2 (NH, CH, CH_2) or 1.5 (OH, CH_3) times U_{eq} of the parent atom.

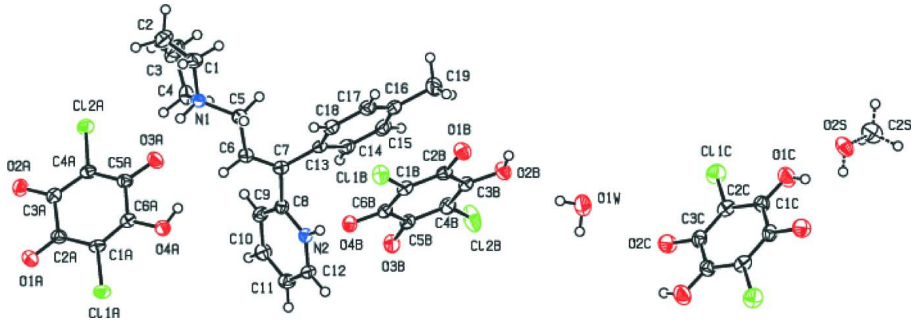

Figure 1

Molecular structure of (I) with the atom labeling scheme. Displacement ellipsoids for non-H atoms are drawn at the 50% probability level. Only the major component of the disorder is shown.

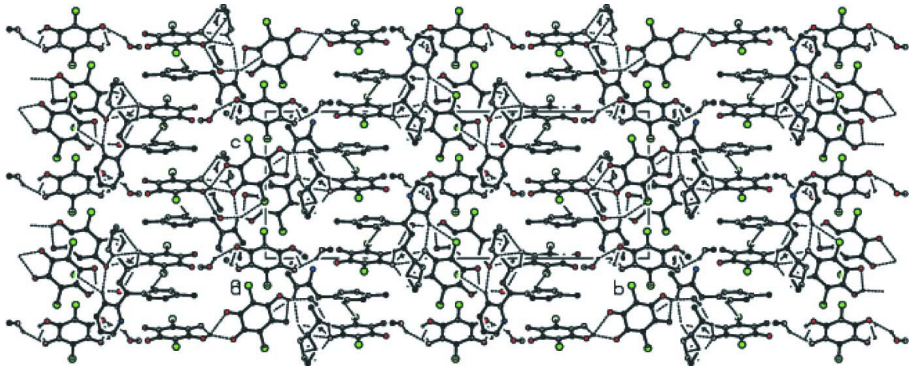

Figure 2

Perspective view of the crystal packing and hydrogen bonding of (I) down the *a* axis. For clarity, hydrogen atoms not involved in hydrogen bonding have been omitted and only the major component of the disorder is shown.

2-[1-(4-methylphenyl)-3-(pyrrolidin-1-ium-1-yl)prop-1-en-1-yl]pyridin-1-ium bis(2,5-dichloro-4-hydroxy-3,6-dioxocyclohexa-1,4-dien-1-olate)–2,5-dichloro- 3,6-dihydroxycyclohexa-2,5-diene-1,4-dione–methanol–water (2/1/2/2)

Crystal data

$C_{19}H_{24}N_2^{2+}·2C_6HCl_2O_4^-·0.5C_6H_2Cl_2O_4·CH_4O·H_2O$
M_r = 850.88

Monoclinic, $P2_1/n$
Hall symbol: -P 2yn

a = 9.1633 (2) Å
b = 32.3720 (7) Å
c = 12.9834 (4) Å
β = 106.685 (3)°
V = 3689.17 (17) Å^3
Z = 4
F(000) = 1752
D_x = 1.532 Mg m^{-3}

Cu $K\alpha$ radiation, λ = 1.54184 Å
Cell parameters from 10725 reflections
θ = 2.7–75.5°
μ = 4.16 mm^{-1}
T = 123 K
Plate, dark brown
0.5 × 0.38 × 0.12 mm

Data collection

Agilent Xcalibur Ruby Gemini diffractometer
Radiation source: Enhance (Cu) X-ray Source
Graphite monochromator
Detector resolution: 10.5081 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2011)
T_{min} = 0.188, T_{max} = 0.607

25133 measured reflections
7532 independent reflections
6721 reflections with $I > 2\sigma(I)$
R_{int} = 0.036
θ_{max} = 75.7°, θ_{min} = 2.7°
h = −9→11
k = −39→40
l = −16→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.137
S = 1.08
7532 reflections
510 parameters
4 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.065P)^2 + 4.4856P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.08 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted R-factors wR and all goodnesses 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 observed criterion of $F^2 > \sigma(F^2)$ is used only for calculating -R-factor-obs *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}	Occ. (<1)
N1	0.6083 (3)	0.38941 (7)	−0.02161 (17)	0.0253 (6)	
N2	0.5846 (2)	0.37690 (6)	0.42666 (17)	0.0219 (6)	
C1	0.6360 (4)	0.36770 (10)	−0.1171 (2)	0.0396 (10)	
C2	0.5318 (5)	0.38991 (13)	−0.2126 (3)	0.0566 (13)	
C3	0.3923 (4)	0.39853 (14)	−0.1786 (3)	0.0562 (13)	
C4	0.4523 (3)	0.40954 (9)	−0.0600 (2)	0.0329 (8)	
C5	0.6297 (3)	0.36064 (8)	0.0717 (2)	0.0256 (7)	
C6	0.5944 (3)	0.38106 (8)	0.1656 (2)	0.0262 (7)	

C7	0.5387 (3)	0.36176 (8)	0.2373 (2)	0.0237 (7)	
C8	0.5085 (3)	0.38700 (7)	0.3248 (2)	0.0229 (7)	
C9	0.4040 (3)	0.41905 (8)	0.3069 (2)	0.0271 (7)	
C10	0.3852 (3)	0.44096 (8)	0.3946 (2)	0.0300 (8)	
C11	0.4688 (3)	0.43054 (8)	0.4977 (2)	0.0279 (8)	
C12	0.5685 (3)	0.39775 (8)	0.5118 (2)	0.0243 (7)	
C13	0.5056 (3)	0.31700 (8)	0.23996 (19)	0.0240 (7)	
C14	0.3774 (3)	0.30343 (9)	0.2686 (2)	0.0302 (8)	
C15	0.3474 (4)	0.26157 (10)	0.2725 (2)	0.0375 (9)	
C16	0.4406 (4)	0.23209 (9)	0.2476 (2)	0.0376 (9)	
C17	0.5687 (4)	0.24541 (9)	0.2205 (2)	0.0346 (8)	
C18	0.6013 (3)	0.28713 (8)	0.2174 (2)	0.0292 (8)	
C19	0.4090 (5)	0.18638 (10)	0.2523 (3)	0.0536 (13)	
Cl1A	1.17727 (7)	0.54478 (2)	0.31560 (5)	0.0301 (2)	
Cl2A	0.65597 (7)	0.50251 (2)	−0.11080 (5)	0.0304 (2)	
O1A	1.0309 (3)	0.60103 (6)	0.13472 (17)	0.0373 (6)	
O2A	0.8198 (2)	0.58421 (6)	−0.05149 (15)	0.0294 (5)	
O3A	0.8213 (2)	0.44654 (6)	0.06840 (16)	0.0326 (6)	
O4A	1.0396 (2)	0.46331 (6)	0.24478 (15)	0.0292 (5)	
C1A	1.0377 (3)	0.53290 (8)	0.1979 (2)	0.0244 (7)	
C2A	0.9846 (3)	0.56589 (8)	0.1210 (2)	0.0240 (7)	
C3A	0.8602 (3)	0.55558 (8)	0.0146 (2)	0.0239 (7)	
C4A	0.8028 (3)	0.51523 (8)	0.00329 (19)	0.0235 (7)	
C5A	0.8605 (3)	0.48339 (8)	0.0769 (2)	0.0236 (7)	
C6A	0.9862 (3)	0.49402 (8)	0.1777 (2)	0.0234 (7)	
Cl1B	0.95280 (7)	0.24300 (2)	0.41301 (6)	0.0322 (2)	
Cl2B	0.38936 (10)	0.23353 (2)	0.60046 (9)	0.0526 (3)	
O1B	0.7894 (2)	0.16893 (6)	0.45954 (17)	0.0319 (6)	
O2B	0.5596 (2)	0.16314 (6)	0.54515 (17)	0.0314 (6)	
O3B	0.5501 (2)	0.30750 (6)	0.55902 (17)	0.0323 (6)	
O4B	0.7820 (2)	0.31432 (5)	0.47158 (15)	0.0257 (5)	
C1B	0.7997 (3)	0.24176 (8)	0.46650 (19)	0.0229 (7)	
C2B	0.7414 (3)	0.20213 (8)	0.48159 (19)	0.0236 (7)	
C3B	0.6074 (3)	0.20037 (8)	0.5271 (2)	0.0252 (7)	
C4B	0.5425 (3)	0.23515 (8)	0.5487 (2)	0.0275 (7)	
C5B	0.6020 (3)	0.27584 (8)	0.5340 (2)	0.0244 (7)	
C6B	0.7379 (3)	0.27837 (8)	0.48720 (19)	0.0227 (7)	
Cl1C	0.18813 (8)	0.00452 (2)	0.81624 (6)	0.0405 (2)	
O1C	0.3493 (3)	−0.07006 (7)	0.92826 (19)	0.0422 (7)	
O2C	0.3816 (3)	0.07432 (6)	0.92023 (18)	0.0380 (6)	
C1C	0.4153 (3)	−0.03683 (8)	0.9587 (2)	0.0279 (8)	
C2C	0.3582 (3)	0.00227 (9)	0.9176 (2)	0.0287 (7)	
C3C	0.4335 (3)	0.03859 (8)	0.9551 (2)	0.0275 (7)	
O1S	0.5299 (3)	0.14776 (7)	0.9411 (2)	0.0366 (8)	0.836 (4)
C1S	0.6758 (5)	0.16296 (13)	1.0010 (4)	0.0446 (14)	0.836 (4)
O2S	0.4348 (14)	−0.1470 (4)	0.9421 (12)	0.0366 (8)	0.164 (4)
C2S	0.298 (2)	−0.1688 (7)	0.940 (2)	0.0446 (14)	0.164 (4)
O1W	0.4911 (3)	0.11809 (7)	0.7256 (2)	0.0500 (8)	

H1A	0.60940	0.33800	−0.11770	0.0480*	
H1B	0.74380	0.37030	−0.11670	0.0480*	
H1C	0.68020	0.41040	−0.00100	0.0300*	
H2A	0.57880	0.41590	−0.22770	0.0680*	
H2B	0.50750	0.37220	−0.27750	0.0680*	
H2C	0.64740	0.35570	0.43770	0.0260*	
H3A	0.32570	0.37390	−0.18890	0.0670*	
H3B	0.33380	0.42180	−0.22020	0.0670*	
H4A	0.46070	0.43990	−0.05030	0.0390*	
H4B	0.38390	0.39870	−0.01960	0.0390*	
H5A	0.73630	0.35070	0.09410	0.0310*	
H5B	0.56230	0.33640	0.04910	0.0310*	
H6A	0.61320	0.40990	0.17490	0.0310*	
H9A	0.34600	0.42600	0.23580	0.0330*	
H10A	0.31460	0.46310	0.38340	0.0360*	
H11A	0.45790	0.44570	0.55770	0.0330*	
H12A	0.62610	0.38990	0.58230	0.0290*	
H14A	0.31060	0.32300	0.28540	0.0360*	
H15A	0.26040	0.25300	0.29280	0.0450*	
H17A	0.63510	0.22560	0.20370	0.0410*	
H18A	0.69050	0.29550	0.19960	0.0350*	
H19A	0.33110	0.18210	0.28950	0.0800*	
H19B	0.50290	0.17210	0.29140	0.0800*	
H19C	0.37270	0.17530	0.17910	0.0800*	
H4AA	0.99890	0.44110	0.21770	0.0350*	
H2BA	0.60650	0.14510	0.52060	0.0380*	
H2CA	0.44580	0.09250	0.94910	0.0460*	0.53 (6)
H1CA	0.40330	−0.08970	0.96060	0.0510*	0.47 (6)
H1S	0.46160	0.16340	0.95050	0.0550*	0.836 (4)
H1S1	0.75540	0.14480	0.98980	0.0670*	0.836 (4)
H1S2	0.68210	0.16350	1.07760	0.0670*	0.836 (4)
H1S3	0.68990	0.19100	0.97680	0.0670*	0.836 (4)
H2S	0.46300	−0.13290	0.99860	0.0550*	0.164 (4)
H2S1	0.21600	−0.14900	0.93630	0.0670*	0.164 (4)
H2S2	0.31540	−0.18550	1.00540	0.0670*	0.164 (4)
H2S3	0.26970	−0.18690	0.87690	0.0670*	0.164 (4)
H1W1	0.509 (6)	0.1352 (12)	0.782 (2)	0.0750*	
H1W2	0.526 (6)	0.1329 (12)	0.687 (3)	0.0750*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0281 (11)	0.0271 (10)	0.0237 (10)	−0.0086 (8)	0.0121 (9)	−0.0049 (8)
N2	0.0219 (10)	0.0215 (9)	0.0227 (10)	0.0015 (7)	0.0073 (8)	0.0007 (8)
C1	0.0541 (19)	0.0407 (16)	0.0315 (15)	−0.0100 (14)	0.0243 (14)	−0.0120 (12)
C2	0.078 (3)	0.066 (2)	0.0261 (16)	−0.031 (2)	0.0154 (16)	−0.0012 (15)
C3	0.050 (2)	0.077 (3)	0.0341 (18)	−0.0118 (18)	−0.0001 (15)	0.0200 (17)
C4	0.0323 (14)	0.0280 (13)	0.0394 (15)	−0.0021 (11)	0.0121 (12)	0.0073 (11)

C5	0.0275 (12)	0.0261 (12)	0.0244 (12)	−0.0015 (9)	0.0096 (10)	−0.0012 (9)
C6	0.0305 (13)	0.0247 (12)	0.0245 (12)	−0.0020 (10)	0.0096 (10)	−0.0016 (9)
C7	0.0236 (12)	0.0261 (12)	0.0203 (11)	0.0005 (9)	0.0044 (9)	−0.0019 (9)
C8	0.0239 (12)	0.0241 (11)	0.0215 (12)	−0.0028 (9)	0.0079 (9)	−0.0002 (9)
C9	0.0294 (13)	0.0285 (12)	0.0215 (12)	0.0024 (10)	0.0043 (10)	0.0027 (9)
C10	0.0307 (13)	0.0274 (13)	0.0319 (14)	0.0058 (10)	0.0088 (11)	−0.0001 (10)
C11	0.0284 (13)	0.0302 (13)	0.0265 (13)	−0.0008 (10)	0.0102 (10)	−0.0052 (10)
C12	0.0265 (12)	0.0269 (12)	0.0182 (11)	−0.0021 (9)	0.0043 (9)	−0.0017 (9)
C13	0.0279 (12)	0.0268 (12)	0.0147 (11)	−0.0028 (9)	0.0021 (9)	−0.0002 (9)
C14	0.0309 (13)	0.0359 (14)	0.0217 (12)	−0.0048 (11)	0.0041 (10)	−0.0003 (10)
C15	0.0396 (16)	0.0459 (17)	0.0222 (13)	−0.0172 (13)	0.0013 (11)	0.0051 (11)
C16	0.0557 (19)	0.0297 (14)	0.0180 (12)	−0.0095 (12)	−0.0043 (12)	0.0039 (10)
C17	0.0477 (17)	0.0276 (13)	0.0224 (13)	0.0048 (12)	0.0004 (12)	0.0006 (10)
C18	0.0348 (14)	0.0299 (13)	0.0221 (12)	0.0011 (10)	0.0069 (10)	0.0001 (10)
C19	0.077 (3)	0.0346 (17)	0.0345 (17)	−0.0173 (16)	−0.0076 (16)	0.0073 (13)
Cl1A	0.0304 (3)	0.0339 (3)	0.0225 (3)	−0.0066 (2)	0.0019 (2)	−0.0053 (2)
Cl2A	0.0264 (3)	0.0360 (3)	0.0240 (3)	−0.0046 (2)	−0.0004 (2)	0.0010 (2)
O1A	0.0485 (12)	0.0256 (10)	0.0335 (11)	−0.0067 (8)	0.0051 (9)	−0.0019 (8)
O2A	0.0291 (9)	0.0286 (9)	0.0290 (9)	0.0004 (7)	0.0062 (8)	0.0045 (7)
O3A	0.0330 (10)	0.0255 (9)	0.0342 (10)	−0.0055 (7)	0.0013 (8)	−0.0004 (8)
O4A	0.0310 (10)	0.0265 (9)	0.0253 (9)	−0.0024 (7)	0.0006 (7)	0.0017 (7)
C1A	0.0224 (11)	0.0307 (13)	0.0183 (11)	−0.0014 (9)	0.0031 (9)	−0.0041 (9)
C2A	0.0250 (12)	0.0250 (12)	0.0231 (12)	−0.0016 (9)	0.0088 (10)	−0.0040 (9)
C3A	0.0216 (11)	0.0280 (12)	0.0239 (12)	0.0025 (9)	0.0092 (9)	0.0014 (9)
C4A	0.0190 (11)	0.0301 (12)	0.0198 (11)	−0.0011 (9)	0.0028 (9)	−0.0026 (9)
C5A	0.0218 (11)	0.0265 (12)	0.0230 (12)	−0.0026 (9)	0.0072 (9)	−0.0036 (9)
C6A	0.0219 (11)	0.0284 (12)	0.0199 (11)	0.0007 (9)	0.0062 (9)	0.0003 (9)
Cl1B	0.0295 (3)	0.0312 (3)	0.0419 (4)	0.0047 (2)	0.0199 (3)	0.0024 (3)
Cl2B	0.0561 (5)	0.0320 (4)	0.0915 (7)	0.0010 (3)	0.0562 (5)	0.0018 (4)
O1B	0.0337 (10)	0.0257 (9)	0.0384 (11)	0.0038 (7)	0.0135 (8)	−0.0029 (8)
O2B	0.0343 (10)	0.0238 (9)	0.0406 (11)	−0.0008 (7)	0.0181 (9)	−0.0023 (8)
O3B	0.0374 (10)	0.0271 (9)	0.0386 (11)	0.0042 (8)	0.0209 (9)	0.0011 (8)
O4B	0.0252 (9)	0.0242 (9)	0.0280 (9)	0.0027 (7)	0.0083 (7)	0.0028 (7)
C1B	0.0190 (11)	0.0303 (13)	0.0198 (11)	0.0030 (9)	0.0060 (9)	0.0008 (9)
C2B	0.0217 (11)	0.0278 (12)	0.0191 (11)	0.0050 (9)	0.0025 (9)	−0.0003 (9)
C3B	0.0274 (12)	0.0262 (12)	0.0203 (12)	0.0001 (9)	0.0043 (10)	0.0013 (9)
C4B	0.0256 (12)	0.0321 (13)	0.0278 (13)	0.0007 (10)	0.0125 (10)	0.0010 (10)
C5B	0.0260 (12)	0.0267 (12)	0.0201 (11)	0.0043 (9)	0.0061 (10)	0.0022 (9)
C6B	0.0209 (11)	0.0274 (12)	0.0178 (11)	0.0018 (9)	0.0025 (9)	0.0021 (9)
Cl1C	0.0273 (3)	0.0485 (4)	0.0392 (4)	−0.0011 (3)	−0.0006 (3)	0.0051 (3)
O1C	0.0395 (12)	0.0353 (11)	0.0474 (13)	−0.0103 (9)	0.0055 (10)	0.0020 (9)
O2C	0.0399 (11)	0.0314 (10)	0.0379 (11)	0.0089 (8)	0.0037 (9)	0.0012 (8)
C1C	0.0278 (13)	0.0277 (13)	0.0304 (13)	−0.0035 (10)	0.0118 (11)	−0.0012 (10)
C2C	0.0196 (11)	0.0412 (15)	0.0248 (12)	0.0004 (10)	0.0057 (10)	0.0015 (10)
C3C	0.0291 (13)	0.0266 (12)	0.0296 (13)	0.0037 (10)	0.0131 (11)	0.0040 (10)
O1S	0.0376 (13)	0.0251 (11)	0.0524 (15)	−0.0004 (9)	0.0216 (11)	−0.0056 (10)
C1S	0.037 (2)	0.041 (2)	0.051 (3)	0.0043 (15)	0.0052 (19)	−0.0026 (19)
O2S	0.0376 (13)	0.0251 (11)	0.0524 (15)	−0.0004 (9)	0.0216 (11)	−0.0056 (10)

C2S	0.037 (2)	0.041 (2)	0.051 (3)	0.0043 (15)	0.0052 (19)	−0.0026 (19)
O1W	0.0708 (17)	0.0330 (11)	0.0515 (15)	−0.0025 (11)	0.0260 (13)	0.0042 (10)

Geometric parameters (Å, º)

Cl1A—C1A	1.731 (3)	C16—C17	1.387 (5)
Cl2A—C4A	1.741 (3)	C16—C19	1.512 (4)
Cl1B—C1B	1.735 (3)	C17—C18	1.386 (4)
Cl2B—C4B	1.722 (3)	C1—H1A	0.9900
Cl1C—C2C	1.729 (3)	C1—H1B	0.9900
O1A—C2A	1.209 (3)	C2—H2A	0.9900
O2A—C3A	1.245 (3)	C2—H2B	0.9900
O3A—C5A	1.242 (3)	C3—H3A	0.9900
O4A—C6A	1.320 (3)	C3—H3B	0.9900
O4A—H4AA	0.8400	C4—H4A	0.9900
O1B—C2B	1.226 (3)	C4—H4B	0.9900
O2B—C3B	1.326 (3)	C5—H5A	0.9900
O3B—C5B	1.213 (3)	C5—H5B	0.9900
O4B—C6B	1.267 (3)	C6—H6A	0.9500
O2B—H2BA	0.8400	C9—H9A	0.9500
O1C—C1C	1.242 (4)	C10—H10A	0.9500
O2C—C3C	1.283 (3)	C11—H11A	0.9500
O1C—H1CA	0.8400	C12—H12A	0.9500
O2C—H2CA	0.8400	C14—H14A	0.9500
O1S—C1S	1.427 (6)	C15—H15A	0.9500
O1S—H1S	0.8400	C17—H17A	0.9500
N1—C5	1.496 (3)	C18—H18A	0.9500
N1—C4	1.519 (4)	C19—H19A	0.9800
N1—C1	1.509 (4)	C19—H19C	0.9800
N2—C8	1.346 (3)	C19—H19B	0.9800
N2—C12	1.339 (3)	C1A—C6A	1.343 (4)
O2S—C2S	1.43 (2)	C1A—C2A	1.448 (4)
N1—H1C	0.9300	C2A—C3A	1.554 (4)
N2—H2C	0.8800	C3A—C4A	1.400 (4)
O2S—H2S	0.8400	C4A—C5A	1.402 (4)
O1W—H1W2	0.82 (5)	C5A—C6A	1.514 (4)
O1W—H1W1	0.90 (3)	C1B—C6B	1.373 (4)
C1—C2	1.512 (5)	C1B—C2B	1.425 (4)
C2—C3	1.494 (6)	C2B—C3B	1.509 (4)
C3—C4	1.521 (5)	C3B—C4B	1.340 (4)
C5—C6	1.501 (4)	C4B—C5B	1.459 (4)
C6—C7	1.338 (4)	C5B—C6B	1.537 (4)
C7—C13	1.483 (4)	C1C—C3C^{i}	1.512 (4)
C7—C8	1.488 (4)	C1C—C2C	1.414 (4)
C8—C9	1.386 (4)	C2C—C3C	1.379 (4)
C9—C10	1.394 (4)	C1S—H1S1	0.9800
C10—C11	1.380 (4)	C1S—H1S2	0.9800
C11—C12	1.378 (4)	C1S—H1S3	0.9800

C13—C18	1.392 (4)	C2S—H2S3	0.9800
C13—C14	1.401 (4)	C2S—H2S1	0.9800
C14—C15	1.387 (4)	C2S—H2S2	0.9800
C15—C16	1.380 (5)		

C6A—O4A—H4AA	109.00	C10—C11—H11A	121.00
C3B—O2B—H2BA	109.00	C11—C12—H12A	120.00
C1C—O1C—H1CA	109.00	N2—C12—H12A	120.00
C3C—O2C—H2CA	109.00	C13—C14—H14A	120.00
C1S—O1S—H1S	109.00	C15—C14—H14A	120.00
C4—N1—C5	115.2 (2)	C16—C15—H15A	119.00
C1—N1—C4	107.1 (2)	C14—C15—H15A	119.00
C1—N1—C5	111.2 (2)	C18—C17—H17A	120.00
C8—N2—C12	122.7 (2)	C16—C17—H17A	119.00
C5—N1—H1C	108.00	C17—C18—H18A	119.00
C4—N1—H1C	108.00	C13—C18—H18A	119.00
C1—N1—H1C	108.00	H19A—C19—H19C	109.00
C12—N2—H2C	119.00	C16—C19—H19B	109.00
C8—N2—H2C	119.00	C16—C19—H19C	110.00
C2S—O2S—H2S	109.00	H19A—C19—H19B	109.00
H1W1—O1W—H1W2	97 (4)	H19B—C19—H19C	109.00
N1—C1—C2	103.7 (3)	C16—C19—H19A	109.00
C1—C2—C3	103.8 (3)	Cl1A—C1A—C2A	117.51 (19)
C2—C3—C4	104.6 (3)	C2A—C1A—C6A	121.8 (2)
N1—C4—C3	105.3 (2)	Cl1A—C1A—C6A	120.6 (2)
N1—C5—C6	112.0 (2)	C1A—C2A—C3A	118.1 (2)
C5—C6—C7	125.0 (2)	O1A—C2A—C3A	118.0 (2)
C6—C7—C13	126.4 (2)	O1A—C2A—C1A	123.9 (2)
C8—C7—C13	115.8 (2)	O2A—C3A—C4A	126.4 (2)
C6—C7—C8	117.8 (2)	C2A—C3A—C4A	116.8 (2)
N2—C8—C9	119.0 (2)	O2A—C3A—C2A	116.7 (2)
C7—C8—C9	123.7 (2)	Cl2A—C4A—C3A	119.03 (19)
N2—C8—C7	117.3 (2)	C3A—C4A—C5A	123.9 (2)
C8—C9—C10	119.1 (2)	Cl2A—C4A—C5A	117.0 (2)
C9—C10—C11	120.3 (2)	O3A—C5A—C6A	115.1 (2)
C10—C11—C12	118.7 (2)	C4A—C5A—C6A	117.8 (2)
N2—C12—C11	120.3 (2)	O3A—C5A—C4A	127.1 (2)
C7—C13—C14	120.4 (2)	O4A—C6A—C5A	116.4 (2)
C7—C13—C18	121.9 (2)	C1A—C6A—C5A	121.3 (2)
C14—C13—C18	117.7 (2)	O4A—C6A—C1A	122.3 (2)
C13—C14—C15	120.4 (3)	C2B—C1B—C6B	123.9 (3)
C14—C15—C16	121.7 (3)	Cl1B—C1B—C6B	119.0 (2)
C15—C16—C19	121.9 (3)	Cl1B—C1B—C2B	117.0 (2)
C17—C16—C19	120.0 (3)	O1B—C2B—C3B	116.4 (2)
C15—C16—C17	118.1 (3)	C1B—C2B—C3B	117.9 (2)
C16—C17—C18	121.0 (3)	O1B—C2B—C1B	125.7 (3)
C13—C18—C17	121.1 (3)	C2B—C3B—C4B	120.7 (2)
N1—C1—H1A	111.00	O2B—C3B—C4B	122.5 (3)

C2—C1—H1A	111.00	O2B—C3B—C2B	116.8 (2)
H1A—C1—H1B	109.00	Cl2B—C4B—C3B	121.1 (2)
N1—C1—H1B	111.00	Cl2B—C4B—C5B	117.1 (2)
C2—C1—H1B	111.00	C3B—C4B—C5B	121.8 (3)
C3—C2—H2A	111.00	C4B—C5B—C6B	118.4 (2)
C1—C2—H2B	111.00	O3B—C5B—C6B	119.1 (2)
C1—C2—H2A	111.00	O3B—C5B—C4B	122.5 (3)
H2A—C2—H2B	109.00	C1B—C6B—C5B	117.3 (2)
C3—C2—H2B	111.00	O4B—C6B—C5B	116.4 (2)
C4—C3—H3B	111.00	O4B—C6B—C1B	126.4 (3)
H3A—C3—H3B	109.00	O1C—C1C—C2C	124.2 (3)
C2—C3—H3A	111.00	C2C—C1C—C3C^{i}	118.3 (2)
C4—C3—H3A	111.00	O1C—C1C—C3C^{i}	117.5 (2)
C2—C3—H3B	111.00	C1C—C2C—C3C	122.4 (2)
C3—C4—H4B	111.00	Cl1C—C2C—C3C	118.9 (2)
C3—C4—H4A	111.00	Cl1C—C2C—C1C	118.7 (2)
N1—C4—H4A	111.00	C1C^{i}—C3C—C2C	119.2 (2)
H4A—C4—H4B	109.00	O2C—C3C—C2C	123.2 (3)
N1—C4—H4B	111.00	O2C—C3C—C1C^{i}	117.6 (2)
H5A—C5—H5B	108.00	O1S—C1S—H1S3	109.00
C6—C5—H5A	109.00	O1S—C1S—H1S1	109.00
N1—C5—H5B	109.00	O1S—C1S—H1S2	109.00
C6—C5—H5B	109.00	H1S2—C1S—H1S3	109.00
N1—C5—H5A	109.00	H1S1—C1S—H1S2	109.00
C7—C6—H6A	117.00	H1S1—C1S—H1S3	110.00
C5—C6—H6A	118.00	O2S—C2S—H2S2	109.00
C10—C9—H9A	120.00	O2S—C2S—H2S3	109.00
C8—C9—H9A	120.00	O2S—C2S—H2S1	110.00
C11—C10—H10A	120.00	H2S1—C2S—H2S3	110.00
C9—C10—H10A	120.00	H2S2—C2S—H2S3	109.00
C12—C11—H11A	121.00	H2S1—C2S—H2S2	110.00

C4—N1—C1—C2	22.8 (3)	C1A—C2A—C3A—C4A	3.1 (4)
C5—N1—C1—C2	149.4 (3)	O2A—C3A—C4A—Cl2A	−2.3 (4)
C1—N1—C4—C3	0.4 (3)	O2A—C3A—C4A—C5A	175.1 (3)
C5—N1—C4—C3	−123.9 (3)	C2A—C3A—C4A—Cl2A	176.54 (19)
C1—N1—C5—C6	−176.9 (2)	C2A—C3A—C4A—C5A	−6.1 (4)
C4—N1—C5—C6	−54.8 (3)	Cl2A—C4A—C5A—O3A	2.2 (4)
C8—N2—C12—C11	1.3 (4)	Cl2A—C4A—C5A—C6A	−178.9 (2)
C12—N2—C8—C7	179.0 (2)	C3A—C4A—C5A—O3A	−175.2 (3)
C12—N2—C8—C9	−3.0 (4)	C3A—C4A—C5A—C6A	3.7 (4)
N1—C1—C2—C3	−37.7 (4)	O3A—C5A—C6A—O4A	−0.1 (4)
C1—C2—C3—C4	38.2 (4)	O3A—C5A—C6A—C1A	−178.9 (3)
C2—C3—C4—N1	−23.8 (4)	C4A—C5A—C6A—O4A	−179.1 (2)
N1—C5—C6—C7	149.1 (3)	C4A—C5A—C6A—C1A	2.1 (4)
C5—C6—C7—C8	−179.2 (2)	Cl1B—C1B—C2B—O1B	−0.4 (4)
C5—C6—C7—C13	1.9 (5)	Cl1B—C1B—C2B—C3B	−179.48 (18)
C13—C7—C8—C9	−118.6 (3)	C6B—C1B—C2B—O1B	176.6 (3)

C6—C7—C13—C14	−142.1 (3)	C6B—C1B—C2B—C3B	−2.5 (4)
C6—C7—C13—C18	39.7 (4)	Cl1B—C1B—C6B—O4B	−0.4 (4)
C8—C7—C13—C14	39.0 (3)	Cl1B—C1B—C6B—C5B	179.70 (18)
C8—C7—C13—C18	−139.2 (3)	C2B—C1B—C6B—O4B	−177.3 (2)
C6—C7—C8—C9	62.4 (4)	C2B—C1B—C6B—C5B	2.7 (4)
C13—C7—C8—N2	59.3 (3)	O1B—C2B—C3B—O2B	3.9 (3)
C6—C7—C8—N2	−119.7 (3)	O1B—C2B—C3B—C4B	−176.7 (2)
N2—C8—C9—C10	2.6 (4)	C1B—C2B—C3B—O2B	−176.9 (2)
C7—C8—C9—C10	−179.5 (3)	C1B—C2B—C3B—C4B	2.4 (4)
C8—C9—C10—C11	−0.5 (4)	O2B—C3B—C4B—Cl2B	−0.8 (4)
C9—C10—C11—C12	−1.1 (4)	O2B—C3B—C4B—C5B	176.5 (2)
C10—C11—C12—N2	0.8 (4)	C2B—C3B—C4B—Cl2B	179.9 (2)
C7—C13—C14—C15	−179.2 (2)	C2B—C3B—C4B—C5B	−2.8 (4)
C18—C13—C14—C15	−0.9 (4)	Cl2B—C4B—C5B—O3B	1.8 (4)
C7—C13—C18—C17	179.9 (2)	Cl2B—C4B—C5B—C6B	−179.56 (18)
C14—C13—C18—C17	1.6 (4)	C3B—C4B—C5B—O3B	−175.6 (3)
C13—C14—C15—C16	−0.7 (4)	C3B—C4B—C5B—C6B	3.0 (4)
C14—C15—C16—C17	1.4 (4)	O3B—C5B—C6B—O4B	−4.1 (4)
C14—C15—C16—C19	179.7 (3)	O3B—C5B—C6B—C1B	175.8 (2)
C15—C16—C17—C18	−0.7 (4)	C4B—C5B—C6B—O4B	177.2 (2)
C19—C16—C17—C18	−178.9 (3)	C4B—C5B—C6B—C1B	−2.9 (3)
C16—C17—C18—C13	−0.9 (4)	O1C—C1C—C2C—Cl1C	−1.6 (4)
Cl1A—C1A—C2A—O1A	−0.7 (4)	O1C—C1C—C2C—C3C	178.6 (3)
Cl1A—C1A—C2A—C3A	179.5 (2)	C3C^{i}—C1C—C2C—Cl1C	178.13 (19)
C6A—C1A—C2A—O1A	−177.9 (3)	C3C^{i}—C1C—C2C—C3C	−1.6 (4)
C6A—C1A—C2A—C3A	2.3 (4)	O1C—C1C—C3C^{i}—O2C^{i}	1.2 (4)
Cl1A—C1A—C6A—O4A	−0.8 (4)	O1C—C1C—C3C^{i}—C2C^{i}	−178.7 (3)
Cl1A—C1A—C6A—C5A	177.9 (2)	C2C—C1C—C3C^{i}—O2C^{i}	−178.6 (3)
C2A—C1A—C6A—O4A	176.4 (3)	C2C—C1C—C3C^{i}—C2C^{i}	1.5 (4)
C2A—C1A—C6A—C5A	−4.9 (4)	Cl1C—C2C—C3C—O2C	1.8 (4)
O1A—C2A—C3A—O2A	2.3 (4)	Cl1C—C2C—C3C—C1C^{i}	−178.1 (2)
O1A—C2A—C3A—C4A	−176.7 (3)	C1C—C2C—C3C—O2C	−178.5 (3)
C1A—C2A—C3A—O2A	−178.0 (2)	C1C—C2C—C3C—C1C^{i}	1.6 (4)

Symmetry code: (i) −*x*+1, −*y*, −*z*+2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4*A*—H4*AA*···O3*A*	0.84	2.15	2.629 (3)	116
O4*A*—H4*AA*···O1*W*^{ii}	0.84	1.92	2.672 (3)	148
N1—H1*C*···O3*A*	0.93	1.78	2.699 (3)	167
O2*B*—H2*BA*···O1*B*	0.84	2.19	2.655 (3)	115
O2*B*—H2*BA*···O1*A*^{iii}	0.84	2.50	3.012 (3)	121
O2*B*—H2*BA*···O2*A*^{iii}	0.84	2.08	2.776 (3)	139
N2—H2*C*···O3*B*	0.88	2.55	2.900 (3)	104
N2—H2*C*···O4*B*	0.88	1.79	2.667 (3)	175
O2*C*—H2*CA*···O1*C*^{i}	0.84	2.21	2.680 (4)	116

O1*W*—H1*W*1···O1*S*	0.90 (3)	2.06 (3)	2.882 (3)	152 (4)
O1*W*—H1*W*2···O2*B*	0.82 (5)	2.18 (4)	2.976 (3)	162 (4)
C1—H1*B*···O1*A*^{iv}	0.99	2.34	3.286 (5)	160
C3—H3*A*···O1*B*^{v}	0.99	2.47	3.138 (5)	124
C4—H4*B*···O2*A*^{vi}	0.99	2.37	3.229 (3)	144
C4—H4*B*···O1*B*^{v}	0.99	2.34	2.994 (3)	123
C5—H5*B*···O1*B*^{v}	0.99	2.44	3.186 (3)	132
C9—H9*A*···Cl2*A*^{vi}	0.95	2.82	3.525 (3)	131
C9—H9*A*···O2*A*^{vi}	0.95	2.46	3.363 (3)	158
C18—H18*A*···Cl2*B*^{ii}	0.95	2.68	3.467 (3)	140
C19—H19*B*···O1*A*^{iii}	0.98	2.55	3.102 (4)	116

Symmetry codes: (i) −*x*+1, −*y*, −*z*+2; (ii) *x*+1/2, −*y*+1/2, *z*−1/2; (iii) −*x*+3/2, *y*−1/2, −*z*+1/2; (iv) −*x*+2, −*y*+1, −*z*; (v) *x*−1/2, −*y*+1/2, *z*−1/2; (vi) −*x*+1, −*y*+1, −*z*.