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2-{1-[2-((2-Ammonioethyl){2-[1-(5-chloro-2-hydroxyphenyl)ethylideneamino]ethyl}amino)ethyliminio]ethyl}-4-chlorophenolate trifluoroacetate

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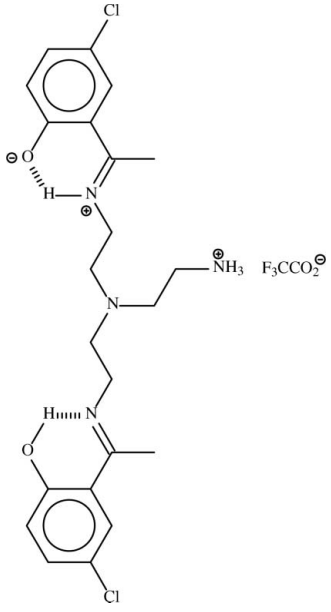
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; R factor = 0.048; wR factor = 0.126; data-to-parameter ratio = 16.2.

In the title ion-pair, $C_{22}H_{29}Cl_2N_4O_2^+\cdot C_2F_3O_2^-$, ammonium–carboxylate N—H···O hydrogen bonds link two cations and two anions about a centre of inversion to generate a hydrogen-bonded tetramer. In the cation, one of the imino N atoms is protonated and donates a hydrogen bond to the O atom of the adjacent chlorophenyl ring. The other imino N atom acts as a hydrogen-bond acceptor from a phenolate O atom.

Related literature

The precursor Schiff base, bis{2-[1-(5-chloro-2-hydroxyphenyl)ethyleneamino]ethyl}{2-[1-(5-chloro-2-phenolate)-ethyleneaminio]ethyl}amine, has one of the three C=N double bonds protonated on the N atom (Lee *et al.*, 2009).



Experimental

Crystal data

$C_{22}H_{29}Cl_2N_4O_2^+\cdot C_2F_3O_2^-$
M_r = 565.41
Triclinic, $P\overline{1}$
a = 10.1041 (2) Å
b = 10.6788 (2) Å
c = 12.5241 (3) Å
α = 88.386 (1)°
β = 70.743 (1)°
γ = 81.234 (2)°
V = 1260.48 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.32 mm^{-1}
T = 100 (2) K
0.06 × 0.04 × 0.02 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.981, T_{max} = 0.994
12201 measured reflections
5762 independent reflections
4104 reflections with $I > 2\sigma(I)$
R_{int} = 0.032

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.126
S = 1.03
5762 reflections
356 parameters
5 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.72 e Å^{-3}
$\Delta\rho_{min}$ = −0.46 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H21···N2	0.85 (1)	1.68 (2)	2.493 (2)	159 (4)
N1—H11···O1	0.89 (1)	1.73 (2)	2.520 (2)	147 (3)
N4—H41···O1	0.88 (1)	1.88 (1)	2.742 (2)	168 (2)
N4—H42···O3	0.89 (1)	1.89 (1)	2.769 (3)	169 (3)
N4—H43···O4^{i}	0.89 (1)	1.92 (2)	2.755 (3)	154 (3)

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2856).

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supplementary materials

Acta Cryst. (2009). E**65**, o410 [**doi:10.1107/S1600536809002943**]

2-{1-[2-((2-Ammonioethyl){2-[1-(5-chloro-2-hydroxyphenyl)ethylideneamino]ethyl}amino)ethyliminio]ethyl}-4-chlorophenolate trifluoroacetate

S. M. Lee, H. M. Ali, K. M. Lo and S. W. Ng

Experimental

Tris(2-aminoethyl)amine (1.46 g m 10 mmol) was condensed with 5-chloro-2-hydroxyacetophenone (5.12 g, 30 mol) in refluxing ethanol (100 ml) to yield the unsolvated Schiff base. The compound (0.64 g, 1 mmol) and trifluoroacetic acid (0.11 g, 1 mmol) were dissolved in a small volume of ethanol. Crystals of the salt separated after several days.

Refinement

Carbon-bound H atoms were placed in calculated positions (C—H = 0.93–0.99 Å) and were included in the refinement in the riding model approximation, with *U*(H) set to 1.2 to 1.5*U*(C). The methyl H atoms were rotated to fit the electron density.

The iminium/ammonium and hydroxy H atoms were located in a difference Fourier map, and were refined with distance restraints [N—H = 0.88 (1) and O—H = 0.84 (1) Å; their isotropic displacement parameters were freely refined.

Figures

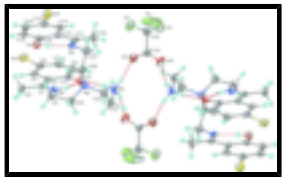


Fig. 1. Anisotropic displacement ellipsoid plot (Barbour, 2001) of the title compound at the 70% probability level. H atoms are drawn as spheres of arbitrary radius.

2-{1-[2-((2-Ammonioethyl){2-[1-(5-chloro-2- hydroxyphenyl)ethylideneamino]ethyl}amino)ethyliminio]ethyl}-4-chlorophenolate trifluoroacetate

Crystal data

$C_{22}H_{29}Cl_2N_4O_2^+ \cdot C_2F_3O_2^-$	$Z = 2$
$M_r = 565.41$	$F_{000} = 588$
Triclinic, $P\overline{1}$	$D_x = 1.490$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 10.1041$ (2) Å	Cell parameters from 2402 reflections
$b = 10.6788$ (2) Å	$\theta = 2.2$–$27.8°$
$c = 12.5241$ (3) Å	$\mu = 0.32$ mm^{-1}
$\alpha = 88.386$ (1)°	$T = 100$ (2) K
$\beta = 70.743$ (1)°	Prism, yellow

γ = 81.234 (2)°	0.06 × 0.04 × 0.02 mm
V = 1260.48 (5) Å^3	

Data collection

Bruker SMART APEX diffractometer	5762 independent reflections
Radiation source: fine-focus sealed tube	4104 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.032
T = 100(2) K	θ_{max} = 27.5°
ω scans	θ_{min} = 1.7°
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −13→13
T_{min} = 0.981, T_{max} = 0.994	k = −13→13
12201 measured reflections	l = −16→16

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.048	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.126	$w = 1/[\sigma^2(F_o^2) + (0.0533P)^2 + 0.6261P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.03	$(\Delta/\sigma)_{max}$ = 0.001
5762 reflections	$\Delta\rho_{max}$ = 0.72 e Å^{-3}
356 parameters	$\Delta\rho_{min}$ = −0.46 e Å^{-3}
5 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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

	x	y	z	U_{iso}*/U_{eq}
Cl1	0.10326 (7)	0.47757 (6)	1.36535 (5)	0.03022 (16)
Cl2	0.46582 (7)	0.29988 (6)	1.26264 (5)	0.03337 (17)
O1	0.24624 (17)	0.42151 (15)	0.87521 (13)	0.0261 (4)
O2	0.22931 (18)	−0.00604 (16)	1.01009 (14)	0.0258 (4)
H21	0.278 (4)	0.005 (4)	0.9419 (14)	0.092 (14)*
O3	0.6309 (2)	0.30567 (19)	0.55587 (16)	0.0445 (5)
O4	0.7436 (2)	0.30693 (16)	0.36975 (14)	0.0349 (4)
N1	0.0653 (2)	0.27355 (18)	0.90939 (15)	0.0203 (4)
H11	0.135 (2)	0.316 (2)	0.871 (2)	0.042 (8)*
N2	0.39560 (19)	0.06404 (17)	0.83106 (15)	0.0214 (4)
N3	0.23242 (19)	0.19477 (17)	0.68450 (15)	0.0207 (4)
N4	0.3612 (2)	0.4419 (2)	0.64538 (17)	0.0242 (4)
H41	0.332 (3)	0.425 (2)	0.7177 (10)	0.027 (7)*

H42	0.4511 (14)	0.408 (2)	0.613 (2)	0.044 (8)*
H43	0.353 (3)	0.5260 (10)	0.641 (2)	0.038 (8)*
C1	0.2076 (2)	0.4375 (2)	0.98379 (18)	0.0200 (5)
C2	0.0963 (2)	0.37800 (19)	1.06063 (18)	0.0177 (4)
C3	0.0633 (2)	0.3952 (2)	1.17817 (18)	0.0193 (5)
H3	−0.0113	0.3569	1.2290	0.023*
C4	0.1376 (2)	0.4664 (2)	1.21953 (18)	0.0216 (5)
C5	0.2434 (2)	0.5277 (2)	1.1471 (2)	0.0247 (5)
H5	0.2925	0.5787	1.1773	0.030*
C6	0.2769 (2)	0.5144 (2)	1.0326 (2)	0.0246 (5)
H6	0.3485	0.5578	0.9842	0.030*
C7	0.0240 (2)	0.2942 (2)	1.01801 (18)	0.0179 (4)
C8	−0.0912 (2)	0.2298 (2)	1.09553 (19)	0.0250 (5)
H8A	−0.1262	0.1773	1.0509	0.037*
H8B	−0.1692	0.2938	1.1394	0.037*
H8C	−0.0539	0.1763	1.1471	0.037*
C9	0.0156 (2)	0.1860 (2)	0.84896 (19)	0.0227 (5)
H9A	−0.0893	0.2016	0.8730	0.027*
H9B	0.0458	0.0976	0.8668	0.027*
C10	0.0773 (2)	0.2056 (2)	0.72269 (19)	0.0231 (5)
H10A	0.0499	0.1418	0.6814	0.028*
H10B	0.0368	0.2906	0.7044	0.028*
C11	0.3915 (2)	0.1380 (2)	1.00730 (18)	0.0193 (5)
C12	0.4442 (2)	0.2098 (2)	1.07147 (19)	0.0214 (5)
H12	0.5183	0.2569	1.0342	0.026*
C13	0.3905 (2)	0.2132 (2)	1.18738 (19)	0.0222 (5)
C14	0.2819 (2)	0.1461 (2)	1.24520 (19)	0.0237 (5)
H14	0.2442	0.1503	1.3255	0.028*
C15	0.2300 (2)	0.0732 (2)	1.18385 (19)	0.0224 (5)
H15	0.1565	0.0261	1.2227	0.027*
C16	0.2827 (2)	0.0670 (2)	1.06586 (19)	0.0208 (5)
C17	0.4476 (2)	0.1367 (2)	0.88267 (19)	0.0214 (5)
C18	0.5569 (3)	0.2198 (2)	0.8265 (2)	0.0273 (5)
H18A	0.5891	0.2051	0.7444	0.041*
H18B	0.6377	0.1995	0.8540	0.041*
H18C	0.5152	0.3089	0.8443	0.041*
C19	0.4354 (3)	0.0499 (2)	0.70858 (19)	0.0259 (5)
H19A	0.4932	−0.0341	0.6833	0.031*
H19B	0.4927	0.1159	0.6711	0.031*
C20	0.3015 (2)	0.0623 (2)	0.6765 (2)	0.0247 (5)
H20A	0.3258	0.0295	0.5981	0.030*
H20B	0.2347	0.0104	0.7273	0.030*
C21	0.2872 (3)	0.2563 (2)	0.57570 (19)	0.0266 (5)
H21A	0.2368	0.2340	0.5249	0.032*
H21B	0.3889	0.2223	0.5404	0.032*
C22	0.2712 (3)	0.3986 (2)	0.5850 (2)	0.0274 (5)
H22A	0.2968	0.4336	0.5081	0.033*
H22B	0.1706	0.4325	0.6256	0.033*
C23	0.7267 (2)	0.2710 (2)	0.4670 (2)	0.0245 (5)

C24	0.8459 (3)	0.1700 (2)	0.4815 (2)	0.0281 (5)
F1	0.79561 (19)	0.07794 (17)	0.54812 (16)	0.0644 (6)
F2	0.9303 (2)	0.21998 (18)	0.5210 (2)	0.0813 (8)
F3	0.92729 (18)	0.11073 (17)	0.38502 (15)	0.0550 (5)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0342 (3)	0.0384 (4)	0.0199 (3)	0.0023 (3)	−0.0144 (3)	−0.0062 (2)
Cl2	0.0386 (4)	0.0377 (4)	0.0288 (3)	−0.0110 (3)	−0.0150 (3)	−0.0050 (3)
O1	0.0300 (9)	0.0305 (9)	0.0170 (8)	−0.0130 (7)	−0.0031 (7)	0.0024 (7)
O2	0.0267 (9)	0.0292 (9)	0.0234 (9)	−0.0125 (7)	−0.0069 (8)	0.0015 (7)
O3	0.0322 (10)	0.0547 (13)	0.0297 (10)	0.0114 (9)	0.0037 (8)	0.0106 (9)
O4	0.0475 (11)	0.0331 (10)	0.0223 (9)	−0.0028 (8)	−0.0111 (8)	0.0062 (7)
N1	0.0228 (10)	0.0221 (10)	0.0169 (9)	−0.0087 (8)	−0.0054 (8)	−0.0002 (7)
N2	0.0216 (10)	0.0239 (10)	0.0186 (9)	−0.0002 (8)	−0.0078 (8)	0.0011 (8)
N3	0.0235 (10)	0.0230 (10)	0.0149 (9)	−0.0012 (8)	−0.0065 (8)	−0.0002 (7)
N4	0.0251 (11)	0.0292 (12)	0.0153 (10)	−0.0029 (9)	−0.0034 (9)	0.0054 (8)
C1	0.0233 (11)	0.0173 (11)	0.0197 (11)	−0.0029 (9)	−0.0076 (9)	0.0027 (8)
C2	0.0183 (11)	0.0156 (10)	0.0199 (11)	−0.0020 (8)	−0.0075 (9)	0.0006 (8)
C3	0.0202 (11)	0.0190 (11)	0.0165 (11)	0.0015 (9)	−0.0050 (9)	0.0007 (8)
C4	0.0269 (12)	0.0216 (11)	0.0174 (11)	0.0016 (9)	−0.0110 (10)	−0.0022 (9)
C5	0.0286 (12)	0.0202 (12)	0.0312 (13)	−0.0046 (9)	−0.0170 (11)	−0.0014 (9)
C6	0.0268 (12)	0.0207 (12)	0.0282 (13)	−0.0095 (9)	−0.0094 (10)	0.0035 (9)
C7	0.0191 (11)	0.0159 (10)	0.0186 (11)	−0.0005 (8)	−0.0071 (9)	0.0003 (8)
C8	0.0282 (12)	0.0281 (13)	0.0196 (11)	−0.0121 (10)	−0.0058 (10)	0.0021 (9)
C9	0.0248 (12)	0.0242 (12)	0.0215 (11)	−0.0074 (9)	−0.0088 (10)	−0.0031 (9)
C10	0.0271 (12)	0.0241 (12)	0.0203 (11)	−0.0028 (9)	−0.0110 (10)	−0.0021 (9)
C11	0.0205 (11)	0.0179 (11)	0.0191 (11)	−0.0013 (9)	−0.0067 (9)	0.0018 (8)
C12	0.0200 (11)	0.0190 (11)	0.0255 (12)	−0.0039 (9)	−0.0075 (10)	0.0032 (9)
C13	0.0236 (12)	0.0211 (12)	0.0237 (12)	−0.0011 (9)	−0.0108 (10)	−0.0017 (9)
C14	0.0245 (12)	0.0256 (12)	0.0179 (11)	0.0009 (9)	−0.0050 (9)	0.0011 (9)
C15	0.0200 (11)	0.0212 (11)	0.0231 (12)	−0.0034 (9)	−0.0033 (9)	0.0034 (9)
C16	0.0179 (11)	0.0207 (11)	0.0234 (12)	−0.0015 (9)	−0.0069 (9)	0.0012 (9)
C17	0.0192 (11)	0.0199 (11)	0.0251 (12)	−0.0013 (9)	−0.0083 (10)	0.0029 (9)
C18	0.0277 (13)	0.0311 (13)	0.0216 (12)	−0.0091 (10)	−0.0046 (10)	0.0049 (10)
C19	0.0283 (13)	0.0291 (13)	0.0182 (11)	0.0023 (10)	−0.0075 (10)	−0.0010 (9)
C20	0.0302 (13)	0.0238 (12)	0.0209 (12)	−0.0009 (10)	−0.0106 (10)	−0.0035 (9)
C21	0.0310 (13)	0.0331 (13)	0.0150 (11)	−0.0018 (10)	−0.0078 (10)	0.0008 (9)
C22	0.0313 (13)	0.0306 (13)	0.0209 (12)	−0.0048 (10)	−0.0097 (10)	0.0075 (10)
C23	0.0244 (12)	0.0243 (12)	0.0239 (12)	−0.0046 (9)	−0.0069 (10)	0.0038 (9)
C24	0.0271 (13)	0.0301 (13)	0.0257 (13)	−0.0042 (10)	−0.0072 (11)	0.0029 (10)
F1	0.0543 (11)	0.0495 (11)	0.0659 (13)	0.0096 (9)	0.0014 (10)	0.0328 (10)
F2	0.0898 (15)	0.0505 (12)	0.143 (2)	0.0103 (10)	−0.0980 (16)	−0.0211 (12)
F3	0.0445 (10)	0.0601 (12)	0.0440 (10)	0.0166 (8)	−0.0026 (8)	−0.0095 (8)

Geometric parameters (Å, °)

Cl1—C4	1.747 (2)	C9—C10	1.518 (3)

Cl2—C13	1.749 (2)	C9—H9A	0.9900
O1—C1	1.294 (3)	C9—H9B	0.9900
O2—C16	1.339 (3)	C10—H10A	0.9900
O2—H21	0.847 (10)	C10—H10B	0.9900
O3—C23	1.231 (3)	C11—C12	1.400 (3)
O4—C23	1.231 (3)	C11—C16	1.419 (3)
N1—C7	1.299 (3)	C11—C17	1.474 (3)
N1—C9	1.460 (3)	C12—C13	1.371 (3)
N1—H11	0.889 (10)	C12—H12	0.9500
N2—C17	1.293 (3)	C13—C14	1.389 (3)
N2—C19	1.458 (3)	C14—C15	1.377 (3)
N3—C10	1.467 (3)	C14—H14	0.9500
N3—C20	1.469 (3)	C15—C16	1.396 (3)
N3—C21	1.469 (3)	C15—H15	0.9500
N4—C22	1.487 (3)	C17—C18	1.501 (3)
N4—H41	0.878 (10)	C18—H18A	0.9800
N4—H42	0.886 (10)	C18—H18B	0.9800
N4—H43	0.892 (10)	C18—H18C	0.9800
C1—C6	1.423 (3)	C19—C20	1.520 (3)
C1—C2	1.436 (3)	C19—H19A	0.9900
C2—C3	1.409 (3)	C19—H19B	0.9900
C2—C7	1.450 (3)	C20—H20A	0.9900
C3—C4	1.365 (3)	C20—H20B	0.9900
C3—H3	0.9500	C21—C22	1.507 (3)
C4—C5	1.391 (3)	C21—H21A	0.9900
C5—C6	1.367 (3)	C21—H21B	0.9900
C5—H5	0.9500	C22—H22A	0.9900
C6—H6	0.9500	C22—H22B	0.9900
C7—C8	1.494 (3)	C23—C24	1.545 (3)
C8—H8A	0.9800	C24—F2	1.299 (3)
C8—H8B	0.9800	C24—F1	1.322 (3)
C8—H8C	0.9800	C24—F3	1.329 (3)
C16—O2—H21	102 (3)	C13—C12—H12	119.5
C7—N1—C9	127.14 (19)	C11—C12—H12	119.5
C7—N1—H11	113.5 (19)	C12—C13—C14	121.3 (2)
C9—N1—H11	119.3 (19)	C12—C13—Cl2	118.69 (18)
C17—N2—C19	124.9 (2)	C14—C13—Cl2	119.96 (18)
C10—N3—C20	112.17 (18)	C15—C14—C13	118.7 (2)
C10—N3—C21	111.60 (18)	C15—C14—H14	120.7
C20—N3—C21	109.93 (18)	C13—C14—H14	120.7
C22—N4—H41	112.4 (17)	C14—C15—C16	121.5 (2)
C22—N4—H42	110.4 (19)	C14—C15—H15	119.2
H41—N4—H42	110 (3)	C16—C15—H15	119.2
C22—N4—H43	107.7 (18)	O2—C16—C15	119.2 (2)
H41—N4—H43	106 (2)	O2—C16—C11	121.3 (2)
H42—N4—H43	109 (3)	C15—C16—C11	119.5 (2)
O1—C1—C6	120.6 (2)	N2—C17—C11	116.1 (2)
O1—C1—C2	122.6 (2)	N2—C17—C18	125.6 (2)
C6—C1—C2	116.8 (2)	C11—C17—C18	118.3 (2)

C3—C2—C1	119.7 (2)	C17—C18—H18A	109.5
C3—C2—C7	119.8 (2)	C17—C18—H18B	109.5
C1—C2—C7	120.32 (19)	H18A—C18—H18B	109.5
C4—C3—C2	120.5 (2)	C17—C18—H18C	109.5
C4—C3—H3	119.8	H18A—C18—H18C	109.5
C2—C3—H3	119.8	H18B—C18—H18C	109.5
C3—C4—C5	121.0 (2)	N2—C19—C20	108.94 (19)
C3—C4—Cl1	119.76 (18)	N2—C19—H19A	109.9
C5—C4—Cl1	119.19 (17)	C20—C19—H19A	109.9
C6—C5—C4	120.0 (2)	N2—C19—H19B	109.9
C6—C5—H5	120.0	C20—C19—H19B	109.9
C4—C5—H5	120.0	H19A—C19—H19B	108.3
C5—C6—C1	121.9 (2)	N3—C20—C19	111.49 (19)
C5—C6—H6	119.0	N3—C20—H20A	109.3
C1—C6—H6	119.0	C19—C20—H20A	109.3
N1—C7—C2	117.78 (19)	N3—C20—H20B	109.3
N1—C7—C8	120.4 (2)	C19—C20—H20B	109.3
C2—C7—C8	121.75 (19)	H20A—C20—H20B	108.0
C7—C8—H8A	109.5	N3—C21—C22	114.00 (19)
C7—C8—H8B	109.5	N3—C21—H21A	108.8
H8A—C8—H8B	109.5	C22—C21—H21A	108.8
C7—C8—H8C	109.5	N3—C21—H21B	108.8
H8A—C8—H8C	109.5	C22—C21—H21B	108.8
H8B—C8—H8C	109.5	H21A—C21—H21B	107.6
N1—C9—C10	109.14 (18)	N4—C22—C21	112.88 (19)
N1—C9—H9A	109.9	N4—C22—H22A	109.0
C10—C9—H9A	109.9	C21—C22—H22A	109.0
N1—C9—H9B	109.9	N4—C22—H22B	109.0
C10—C9—H9B	109.9	C21—C22—H22B	109.0
H9A—C9—H9B	108.3	H22A—C22—H22B	107.8
N3—C10—C9	112.01 (18)	O3—C23—O4	130.0 (2)
N3—C10—H10A	109.2	O3—C23—C24	114.3 (2)
C9—C10—H10A	109.2	O4—C23—C24	115.6 (2)
N3—C10—H10B	109.2	F2—C24—F1	109.2 (2)
C9—C10—H10B	109.2	F2—C24—F3	106.2 (2)
H10A—C10—H10B	107.9	F1—C24—F3	104.2 (2)
C12—C11—C16	118.0 (2)	F2—C24—C23	111.5 (2)
C12—C11—C17	120.8 (2)	F1—C24—C23	112.3 (2)
C16—C11—C17	121.2 (2)	F3—C24—C23	113.1 (2)
C13—C12—C11	121.0 (2)		
O1—C1—C2—C3	177.41 (19)	Cl2—C13—C14—C15	−176.52 (17)
C6—C1—C2—C3	−1.5 (3)	C13—C14—C15—C16	−0.8 (3)
O1—C1—C2—C7	1.2 (3)	C14—C15—C16—O2	179.5 (2)
C6—C1—C2—C7	−177.62 (19)	C14—C15—C16—C11	−0.6 (3)
C1—C2—C3—C4	−1.0 (3)	C12—C11—C16—O2	−178.6 (2)
C7—C2—C3—C4	175.23 (19)	C17—C11—C16—O2	1.6 (3)
C2—C3—C4—C5	2.6 (3)	C12—C11—C16—C15	1.5 (3)
C2—C3—C4—Cl1	−175.57 (16)	C17—C11—C16—C15	−178.3 (2)
C3—C4—C5—C6	−1.7 (3)	C19—N2—C17—C11	179.43 (19)

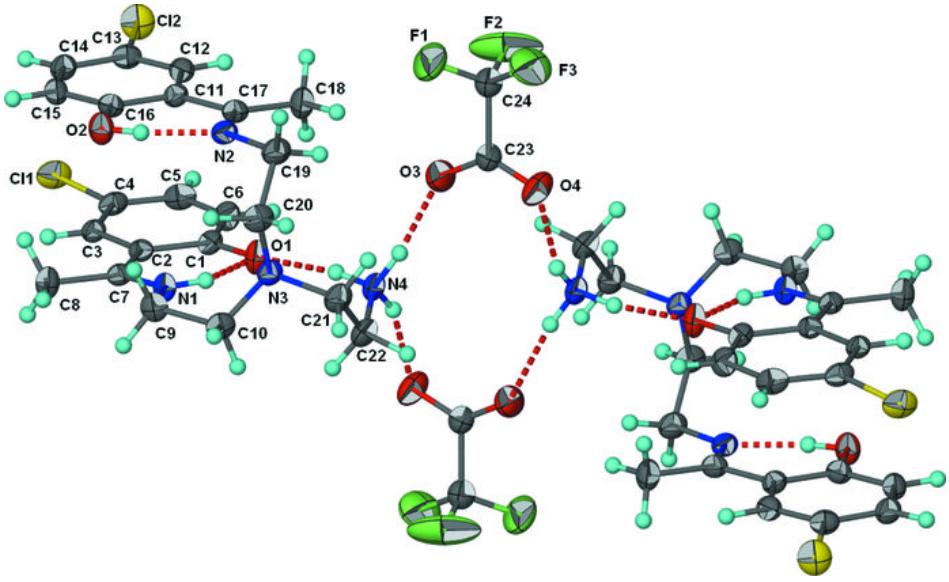
Cl1—C4—C5—C6	176.49 (18)	C19—N2—C17—C18	0.4 (4)
C4—C5—C6—C1	−0.9 (4)	C12—C11—C17—N2	177.7 (2)
O1—C1—C6—C5	−176.5 (2)	C16—C11—C17—N2	−2.5 (3)
C2—C1—C6—C5	2.4 (3)	C12—C11—C17—C18	−3.2 (3)
C9—N1—C7—C2	175.0 (2)	C16—C11—C17—C18	176.6 (2)
C9—N1—C7—C8	−3.1 (3)	C17—N2—C19—C20	−131.8 (2)
C3—C2—C7—N1	−174.86 (19)	C10—N3—C20—C19	−145.03 (19)
C1—C2—C7—N1	1.3 (3)	C21—N3—C20—C19	90.2 (2)
C3—C2—C7—C8	3.3 (3)	N2—C19—C20—N3	74.7 (2)
C1—C2—C7—C8	179.4 (2)	C10—N3—C21—C22	78.2 (2)
C7—N1—C9—C10	172.3 (2)	C20—N3—C21—C22	−156.73 (19)
C20—N3—C10—C9	76.3 (2)	N3—C21—C22—N4	67.2 (3)
C21—N3—C10—C9	−159.79 (18)	O3—C23—C24—F2	−76.8 (3)
N1—C9—C10—N3	54.4 (2)	O4—C23—C24—F2	101.3 (3)
C16—C11—C12—C13	−1.1 (3)	O3—C23—C24—F1	46.1 (3)
C17—C11—C12—C13	178.72 (19)	O4—C23—C24—F1	−135.8 (2)
C11—C12—C13—C14	−0.2 (3)	O3—C23—C24—F3	163.6 (2)
C11—C12—C13—Cl2	177.53 (17)	O4—C23—C24—F3	−18.3 (3)
C12—C13—C14—C15	1.2 (3)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H21···N2	0.85 (1)	1.68 (2)	2.493 (2)	159 (4)
N1—H11···O1	0.89 (1)	1.73 (2)	2.520 (2)	147 (3)
N4—H41···O1	0.88 (1)	1.88 (1)	2.742 (2)	168 (2)
N4—H42···O3	0.89 (1)	1.89 (1)	2.769 (3)	169 (3)
N4—H43···O4^{i}	0.89 (1)	1.92 (2)	2.755 (3)	154 (3)

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

Fig. 1


Cl2
C13
C14
C12
C11
C17
C18
C15
C16
O2
N2
C19
Cl1
C4
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C6
C20
C3
C2
C1
O1
N3
N4
C8
C7
N1
C9
C10
C21
C22
F1
F2
F3
C24
C23
O3
O4