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# (*R*)-1-Phenylethylammonium trifluoroacetate

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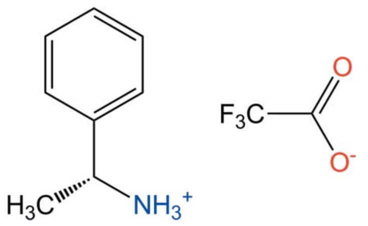
Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.041; $wR$ factor = 0.112; data-to-parameter ratio = 11.6.

In the crystal structure of the title salt, $C_8H_{12}N^+\cdot C_2F_3O_2^-$, all of the ammonium H atoms serve as donors for hydrogen bonds to carboxylate O atoms, forming an $R_4^3(10)$ ring motif based on two cations and two anions. Since both cations and anions act as inter-ion bridging groups, $R(10)$ rings aggregate in a one-dimensional supramolecular network by sharing the strongest N—H···O bond. Edge-sharing motifs lie on the twofold screw axis parallel to [010], and antiparallel packing of these $2_1$-column structural units results in the crystal structure. This arrangement is one of the most commonly occurring in conglomerates of chiral 1-phenylethylamine with achiral monocarboxylic acids, confirming that these ionic salts are particularly robust supramolecular heterosynthons useful in crystal engineering.

## Related literature

For graph-set analysis, see: Etter (1990); Bernstein *et al.* (1995). For characteristic structural patterns found in crystal salts of 1-phenylethylamine and monocarboxylic acids, see: Kinbara, Hashimoto *et al.* (1996); Kinbara, Kai *et al.* (1996); Lemmerer *et al.* (2008). For related chiral salt structures, see: Johansen *et al.* (1998); Boussac *et al.* (2002); Lemmerer *et al.* (2008).



## Experimental

### *Crystal data*

$C_8H_{12}N^+\cdot C_2F_3O_2^-$
$M_r$ = 235.21
Orthorhombic, $P2_12_12_1$
$a$ = 6.7821 (5) Å
$b$ = 6.9887 (8) Å
$c$ = 24.378 (2) Å
$V$ = 1155.49 (19) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.13 mm$^{-1}$
$T$ = 298 K
0.60 × 0.44 × 0.40 mm

### *Data collection*

Siemens P4 diffractometer
3079 measured reflections
1808 independent reflections
1288 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.020
3 standard reflections every 97 reflections
intensity decay: 1%

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.112
$S$ = 1.03
1808 reflections
156 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\rm max}$ = 0.16 e Å$^{-3}$
$\Delta\rho_{\rm min}$ = −0.13 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1$A$···O1 | 0.90 (3) | 1.92 (3) | 2.812 (3) | 171 (3) |
| N1—H1$B$···O2$^{\rm i}$ | 0.92 (3) | 1.97 (3) | 2.818 (3) | 154 (3) |
| N1—H1$C$···O2$^{\rm ii}$ | 0.90 (3) | 1.92 (3) | 2.816 (2) | 175 (3) |

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

Data collection: *XSCANS* (Siemens, 1996); cell refinement: *XSCANS*; data reduction: *XSCANS* (Siemens, 1996); program(s) used to solve structure: *SHELXTL-Plus* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL-Plus*; molecular graphics: *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXTL-Plus*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PB2025).

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# supporting information

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## (*R*)-1-Phenylethylammonium trifluoroacetate

**María-Guadalupe Hernández Linares, Gabriel Guerrero Luna and Sylvain Bernès**

### S1. Comment

In their works about optical resolution of conglomerates, Kinbara *et al.* noted that characteristic hydrogen-bond networks were formed in the salt crystals of 1-phenylethylamine and 1-(4-*iso*propylphenyl)ethylamine with cinnamic acid (Kinbara, Kai *et al.*, 1996). They suggested that "the pattern of hydrogen bonds plays a significant role in the formation of conglomerates" (Kinbara, Hashimoto *et al.*, 1996). In the specific case of salts of chiral 1-phenylethylamine with achiral monocarboxylic acids, a number of structural determinations indeed showed that two predominant supramolecular arrangements are favored by the charge assisted N—H···O hydrogen bonds, which result in crystals belonging to $P2_1$ or $P2_12_12_1$ space groups (Lemmerer *et al.*, 2008): cations and anions associate through quite strong hydrogen bonds to form $C_2^1(4)C_2^2(6)[R_4^3(10)]$ motifs (Etter, 1990; Bernstein *et al.*, 1995). This basic unit has hydrogen bonds with translational units, forming an infinite columnar structure, which generates a screw axis in the crystal structure (invariably a $2_1$ axis). This supramolecular structure, referred as '$2_1$–column' in the Kinbara's reports, may be arranged in a parallel packing in the crystal, which then belongs to $P2_1$ space group, or in an antiparallel fashion, generating $P2_12_12_1$ crystals.

The chiral title salt (Fig. 1) clearly falls in the latter category. Both the cation and anion are placed in general positions in an orthorhombic unit cell. All ammonium H atoms form hydrogen bonds with carboxylate O atoms, giving a ring motif $R_4^3(10)$, as shown in Fig. 2. The strongest hydrogen bond, N1—H1C···O2$^{ii}$ is common to two rings motifs. The repetition of the motif in the [010] direction generates homochiral (*R*)–$2_1$–columns. This 1D supramolecular network includes larger ring motifs, which appear if shared contacts are omitted. The sequence of sub-rings nest is $R_4^3(10) \rightarrow R_6^5(16) \rightarrow R_8^7(22) \rightarrow R_{10}^9(28) \rightarrow \cdots \rightarrow R_{2n}^{2n-1}(6n-2)$ [with $n > 1$]. The shortest contact between neighboring $2_1$–columns is N1—H1B···F2$^{i}$, which should be regarded as a van der Waals contact rather than as an actual hydrogen bond. As a consequence, an antiparallel arrangement of $2_1$–columns is favored (Fig. 2, inset), which is, in turn, reflected in the $P2_12_12_1$ space group. Such crystal structures were obtained for numerous 1-phenylethylamine salts including different anions, *e.g.* bromo-fluoroacetate (Boussac *et al.*, 2002), *m*-iodobenzoate (Lemmerer *et al.*, 2008) or more complex, bulky carboxylate derivatives (Johansen *et al.*, 1998).

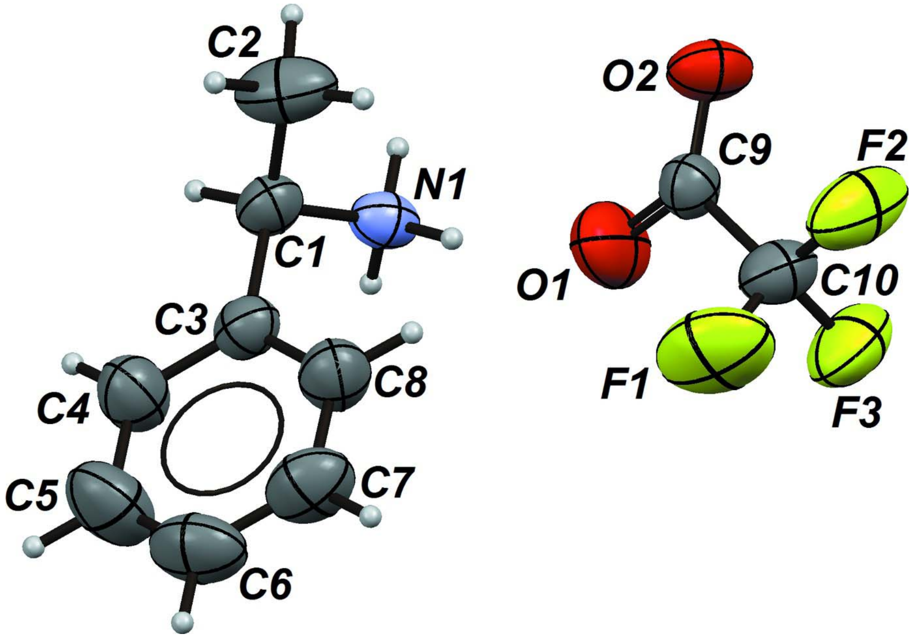
The above description is thus in line with expectations from previous reported structures, and confirms that salts based on chiral 1-phenylethylamine and achiral monocarboxylic acids are robust heterosynthons, useful for crystal engineering and crystal structure prediction. The feature should however not been transferred to other salts (or worse, to cocrystals) of 1-phenylethylamine, which stabilize different supramolecular motifs, if any.

### S2. Experimental

The title salt crystallized when attempting to synthesize a diimine organic ligand. A mixture of (*S*)-6-acetyloxy-5-methyl-2,3-hexanedione (1 g, 5.37 mmol) and $Na_2SO_4$ (4 g) in chloroform (10 ml) was stirred for 5 min. A catalytic amount of trifluoroacetic acid and 2 equiv. of (*R*)-(+)-*α*-phenylethylamine (10.6 mmol) were added and the mixture was refluxed (*ca.* 353 K) under inert atmosphere, until starting materials were not detected by TLC (*ca.* 2 h). After evaporation under reduced pressure, the crude was recrystallized from $CH_2Cl_2$ at 298 K, affording, among other products, the title salt.

## S3. Refinement

As no heavy atoms are present in the crystal and data were measured at room-temperature using Mo *Kα* radiation, no absorption correction was applied to the raw data. Because of insufficient anomalous scattering effects, the Flack parameter could not be reliably determined, and measured Friedel pairs (796) were merged. Absolute configuration was assigned by reference to the chiral amine used as starting material, assuming that no inversion occurred during crystallization. Ammonium H atoms were refined with free coordinates, in order to get accurate dimensions for hydrogen bonds. Other H atoms were placed in idealized positions and refined as riding to their carrier atoms, with bond lengths fixed to 0.93 (aromatic CH), 0.96 (methyl $CH_3$) or 0.98 Å (methine CH). Isotropic displacement parameters for H atoms were calculated as $U_{iso}(H) = 1.2U_{eq}(C)$ for aromatic CH groups and $U_{iso}(H) = 1.5U_{eq}(C, N)$ for other groups. The methyl group was considered as a rigid group free to rotate about its C—C bond.



### Figure 1

The structure of the title compound, with displacement ellipsoids at the 50% probability level for non-H atoms.

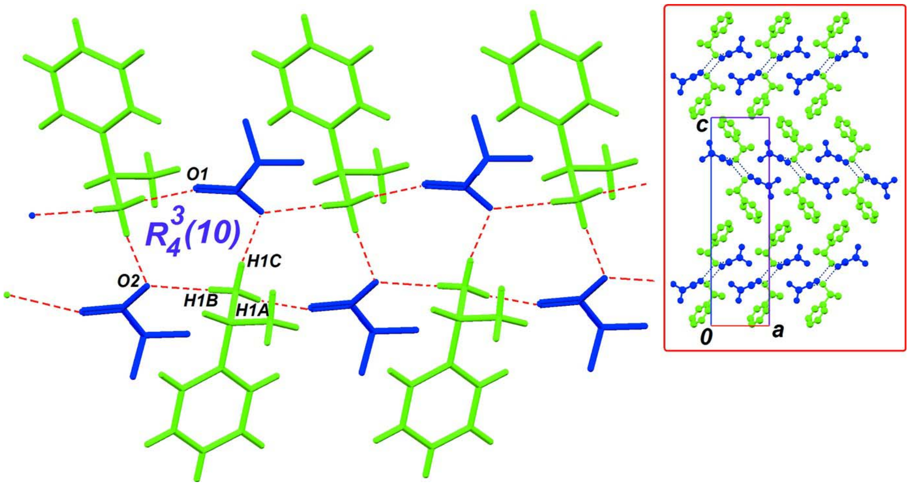


**Figure 2**

The hydrogen-bonding network in the title compound (hydrogen bonds are dashed). The inset represent the packing structure viewed down the axis of the $2_1$–column (*b* axis). H atoms have been omitted for clarity. In both figures, cations are green and anions blue.

## (*R*)-1-Phenylethylammonium trifluoroacetate

### *Crystal data*

$C_8H_{12}N^+\cdot C_2F_3O_2^-$
$M_r = 235.21$
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a = 6.7821$ (5) Å
$b = 6.9887$ (8) Å
$c = 24.378$ (2) Å
$V = 1155.49$ (19) Å$^3$
$Z = 4$
$F(000) = 488$
$D_x = 1.352$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 70 reflections
$\theta = 4.5$–$12.5°$
$\mu = 0.13$ mm$^{-1}$
$T = 298$ K
Prism, colorless
0.60 × 0.44 × 0.40 mm

### *Data collection*

Siemens P4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$2\theta/\omega$ scans
3079 measured reflections
1808 independent reflections
1288 reflections with $I > 2\sigma(I)$
$R_{\text{int}} = 0.020$
$\theta_{\max} = 29.0°$, $\theta_{\min} = 1.7°$
$h = -9 \rightarrow 4$
$k = -9 \rightarrow 1$
$l = -33 \rightarrow 1$
3 standard reflections every 97 reflections
intensity decay: 1%

### *Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.112$
$S = 1.03$
1808 reflections
156 parameters
0 restraints
0 constraints
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

$w = 1/[\sigma^2(F_o^2) + (0.0464P)^2 + 0.1579P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.16$ e Å$^{-3}$
$\Delta\rho_{min} = -0.13$ e Å$^{-3}$

Extinction correction: *SHELXTL-Plus* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.045 (4)

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

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| N1 | 0.9254 (3) | 0.1712 (3) | 0.19995 (7) | 0.0480 (4) |
| H1C | 1.002 (5) | 0.206 (4) | 0.2286 (11) | 0.072* |
| H1B | 0.853 (5) | 0.062 (5) | 0.2039 (11) | 0.072* |
| H1A | 0.840 (5) | 0.268 (5) | 0.1966 (11) | 0.072* |
| C1 | 1.0532 (3) | 0.1429 (4) | 0.15044 (8) | 0.0513 (5) |
| H1 | 1.1377 | 0.0316 | 0.1571 | 0.062* |
| C2 | 1.1846 (5) | 0.3153 (5) | 0.14290 (11) | 0.0818 (9) |
| H2C | 1.2617 | 0.3000 | 0.1102 | 0.123* |
| H2B | 1.2709 | 0.3273 | 0.1739 | 0.123* |
| H2A | 1.1049 | 0.4283 | 0.1398 | 0.123* |
| C3 | 0.9260 (3) | 0.1001 (4) | 0.10055 (8) | 0.0502 (5) |
| C4 | 0.9482 (5) | −0.0721 (4) | 0.07311 (11) | 0.0706 (7) |
| H4 | 1.0390 | −0.1616 | 0.0857 | 0.085* |
| C5 | 0.8359 (6) | −0.1118 (5) | 0.02695 (12) | 0.0893 (10) |
| H5 | 0.8526 | −0.2272 | 0.0086 | 0.107* |
| C6 | 0.7020 (5) | 0.0165 (5) | 0.00854 (11) | 0.0819 (10) |
| H6 | 0.6265 | −0.0114 | −0.0223 | 0.098* |
| C7 | 0.6776 (4) | 0.1863 (5) | 0.03497 (10) | 0.0743 (8) |
| H7 | 0.5859 | 0.2744 | 0.0221 | 0.089* |
| C8 | 0.7891 (4) | 0.2282 (4) | 0.08117 (9) | 0.0633 (7) |
| H8 | 0.7710 | 0.3442 | 0.0992 | 0.076* |
| C9 | 0.6937 (4) | 0.6770 (3) | 0.19540 (9) | 0.0482 (5) |
| O1 | 0.6911 (4) | 0.5019 (3) | 0.19191 (10) | 0.0921 (7) |
| O2 | 0.8190 (3) | 0.7849 (3) | 0.21505 (7) | 0.0620 (5) |
| C10 | 0.5086 (4) | 0.7725 (4) | 0.17224 (11) | 0.0613 (6) |
| F1 | 0.4723 (3) | 0.7214 (4) | 0.12145 (7) | 0.1175 (8) |
| F2 | 0.5178 (3) | 0.9610 (2) | 0.17221 (11) | 0.1065 (8) |
| F3 | 0.3482 (2) | 0.7254 (3) | 0.20053 (8) | 0.0914 (6) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| N1 | 0.0484 (10) | 0.0459 (9) | 0.0498 (9) | −0.0030 (9) | −0.0118 (9) | 0.0002 (9) |
| C1 | 0.0420 (10) | 0.0574 (13) | 0.0545 (11) | 0.0045 (11) | −0.0077 (10) | −0.0010 (10) |
| C2 | 0.0655 (16) | 0.105 (2) | 0.0744 (16) | −0.029 (2) | −0.0104 (14) | 0.0154 (17) |
| C3 | 0.0429 (11) | 0.0622 (13) | 0.0455 (10) | 0.0012 (12) | −0.0017 (9) | 0.0003 (10) |
| C4 | 0.0760 (17) | 0.0669 (16) | 0.0689 (14) | 0.0113 (16) | −0.0136 (15) | −0.0104 (13) |
| C5 | 0.116 (3) | 0.082 (2) | 0.0699 (15) | −0.003 (2) | −0.0199 (18) | −0.0186 (16) |
| C6 | 0.085 (2) | 0.106 (3) | 0.0544 (13) | −0.022 (2) | −0.0162 (15) | −0.0043 (16) |
| C7 | 0.0650 (16) | 0.099 (2) | 0.0585 (13) | 0.0027 (18) | −0.0157 (13) | 0.0114 (15) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C8 | 0.0618 (14) | 0.0706 (16) | 0.0576 (12) | 0.0107 (14) | −0.0108 (12) | −0.0038 (12) |
| C9 | 0.0487 (12) | 0.0465 (12) | 0.0495 (10) | 0.0049 (10) | −0.0017 (10) | −0.0005 (9) |
| O1 | 0.0946 (16) | 0.0488 (11) | 0.1330 (18) | 0.0160 (11) | −0.0199 (16) | −0.0080 (11) |
| O2 | 0.0575 (10) | 0.0609 (10) | 0.0677 (9) | −0.0061 (9) | −0.0241 (8) | 0.0114 (8) |
| C10 | 0.0477 (13) | 0.0611 (14) | 0.0753 (14) | −0.0048 (13) | −0.0089 (12) | 0.0110 (13) |
| F1 | 0.1021 (14) | 0.173 (2) | 0.0768 (10) | −0.0089 (18) | −0.0389 (10) | 0.0115 (13) |
| F2 | 0.0614 (10) | 0.0583 (10) | 0.200 (2) | 0.0064 (9) | −0.0258 (13) | 0.0349 (11) |
| F3 | 0.0526 (8) | 0.0911 (13) | 0.1303 (14) | −0.0024 (10) | 0.0155 (9) | 0.0106 (12) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| N1—C1 | 1.499 (3) | C5—C6 | 1.352 (5) |
| N1—H1C | 0.90 (3) | C5—H5 | 0.9300 |
| N1—H1B | 0.92 (3) | C6—C7 | 1.361 (4) |
| N1—H1A | 0.90 (3) | C6—H6 | 0.9300 |
| C1—C2 | 1.510 (4) | C7—C8 | 1.388 (3) |
| C1—C3 | 1.521 (3) | C7—H7 | 0.9300 |
| C1—H1 | 0.9800 | C8—H8 | 0.9300 |
| C2—H2C | 0.9600 | C9—O1 | 1.227 (3) |
| C2—H2B | 0.9600 | C9—O2 | 1.233 (3) |
| C2—H2A | 0.9600 | C9—C10 | 1.530 (3) |
| C3—C8 | 1.374 (3) | C10—F1 | 1.312 (3) |
| C3—C4 | 1.385 (3) | C10—F2 | 1.319 (3) |
| C4—C5 | 1.387 (4) | C10—F3 | 1.329 (3) |
| C4—H4 | 0.9300 | | |

| | | | |
|---|---|---|---|
| C1—N1—H1C | 109.1 (18) | C5—C4—H4 | 119.8 |
| C1—N1—H1B | 106.6 (18) | C6—C5—C4 | 120.4 (3) |
| H1C—N1—H1B | 117 (2) | C6—C5—H5 | 119.8 |
| C1—N1—H1A | 113.5 (18) | C4—C5—H5 | 119.8 |
| H1C—N1—H1A | 104 (2) | C5—C6—C7 | 120.2 (3) |
| H1B—N1—H1A | 107 (2) | C5—C6—H6 | 119.9 |
| N1—C1—C2 | 109.5 (2) | C7—C6—H6 | 119.9 |
| N1—C1—C3 | 109.99 (17) | C6—C7—C8 | 120.1 (3) |
| C2—C1—C3 | 113.23 (19) | C6—C7—H7 | 119.9 |
| N1—C1—H1 | 108.0 | C8—C7—H7 | 119.9 |
| C2—C1—H1 | 108.0 | C3—C8—C7 | 120.7 (3) |
| C3—C1—H1 | 108.0 | C3—C8—H8 | 119.7 |
| C1—C2—H2C | 109.5 | C7—C8—H8 | 119.7 |
| C1—C2—H2B | 109.5 | O1—C9—O2 | 130.3 (3) |
| H2C—C2—H2B | 109.5 | O1—C9—C10 | 113.4 (2) |
| C1—C2—H2A | 109.5 | O2—C9—C10 | 116.2 (2) |
| H2C—C2—H2A | 109.5 | F1—C10—F2 | 106.3 (2) |
| H2B—C2—H2A | 109.5 | F1—C10—F3 | 105.6 (2) |
| C8—C3—C4 | 118.3 (2) | F2—C10—F3 | 106.6 (3) |
| C8—C3—C1 | 122.0 (2) | F1—C10—C9 | 112.6 (2) |
| C4—C3—C1 | 119.7 (2) | F2—C10—C9 | 113.4 (2) |
| C3—C4—C5 | 120.4 (3) | F3—C10—C9 | 111.85 (19) |

|  |  |  |  |
|---|---|---|---|
| C3—C4—H4 | 119.8 |  |  |
|  |  |  |  |
| N1—C1—C3—C8 | 61.4 (3) | C4—C3—C8—C7 | −0.6 (4) |
| C2—C1—C3—C8 | −61.5 (3) | C1—C3—C8—C7 | 178.9 (2) |
| N1—C1—C3—C4 | −119.1 (2) | C6—C7—C8—C3 | 0.4 (4) |
| C2—C1—C3—C4 | 118.0 (3) | O1—C9—C10—F1 | −54.5 (3) |
| C8—C3—C4—C5 | 0.7 (4) | O2—C9—C10—F1 | 126.5 (2) |
| C1—C3—C4—C5 | −178.8 (3) | O1—C9—C10—F2 | −175.2 (3) |
| C3—C4—C5—C6 | −0.7 (5) | O2—C9—C10—F2 | 5.8 (3) |
| C4—C5—C6—C7 | 0.5 (5) | O1—C9—C10—F3 | 64.2 (3) |
| C5—C6—C7—C8 | −0.4 (5) | O2—C9—C10—F3 | −114.8 (3) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1*A*···O1 | 0.90 (3) | 1.92 (3) | 2.812 (3) | 171 (3) |
| N1—H1*B*···O2$^{i}$ | 0.92 (3) | 1.97 (3) | 2.818 (3) | 154 (3) |
| N1—H1*C*···O2$^{ii}$ | 0.90 (3) | 1.92 (3) | 2.816 (2) | 175 (3) |
| N1—H1*B*···F2$^{i}$ | 0.92 (3) | 2.50 (3) | 3.202 (3) | 134 (2) |

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