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rac-*N*-(6a-Butyl-6-chloro-2-oxoperhydrofuro[3,2-*b*]furan-3-yl)-2,2,2-trifluoroacetamide

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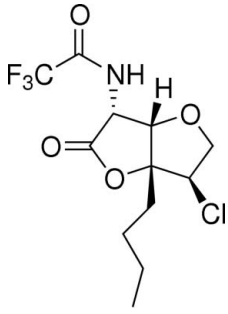
Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.005 Å; disorder in main residue; R factor = 0.031; wR factor = 0.079; data-to-parameter ratio = 12.2.

The title compound, $C_{12}H_{15}ClF_3NO_4$, is a side product in a synthesis of novel furanomycin derivatives. The stereochemistry at the bicyclic core is consistent with a halolactonization step. However, racemization also occurred *via* an unknown mechanism. The five-membered rings are nearly perpendicular to each other [torsion angle at the common bond: −95.6 (2)°].

Related literature

For related literature, see: Erdsack & Krause (2007); Erdsack *et al.* (2007); Hoffmann-Röder & Krause (2001).



Experimental

Crystal data

$C_{12}H_{15}ClF_3NO_4$
M_r = 329.70
Triclinic, $P\overline{1}$
a = 7.674 (3) Å
b = 9.586 (3) Å
c = 11.590 (4) Å
α = 66.904 (13)°
β = 76.782 (14)°
γ = 71.684 (13)°
V = 739.1 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.31 mm^{-1}
T = 291 (1) K
0.10 × 0.08 × 0.08 mm

Data collection

Nonius KappaCCD area-detector diffractometer
Absorption correction: none
8179 measured reflections
2680 independent reflections
959 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.079
S = 0.91
2680 reflections
219 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.12 e Å^{-3}

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* and *SCALEPACK*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1991); software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2450).

References

Erdsack, J. & Krause, N. (2007). *Synthesis*. In preparation.
Erdsack, J., Schürmann, M., Preut, H. & Krause, N. (2007). *Acta Cryst.* E**63**, o664–o665.
Hoffmann-Röder, A. & Krause, N. (2001). *Org. Lett.* **3**, 2537–2538.
Nonius (1998). *COLLECT*. Nonius BV, Delft, The Netherlands.
Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr & R. M. Sweet, pp. 307–326. New York: Academic Press.
Sheldrick, G. M. (1991). *SHELXTL-Plus*. Release 4.1. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

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supplementary materials

Acta Cryst. (2007). E**63**, o3372 [**doi:10.1107/S1600536807031376**]

rac-*N*-(6a-Butyl-6-chloro-2-oxoperhydrofuro[3,2-*b*]furan-3-yl)-2,2,2-trifluoroacetamide

J. Erdsack, M. Schürmann, H. Preut and N. Krause

Comment

The title compound, (I),is a side product in the preparation of novel furanomycin derivatives using the gold-catalyzed cyclization of α-hydroxyallenes (Hoffmann-Röder & Krause, 2001; Erdsack & Krause, 2007) (Fig. 1). The torsion angle O3—C3a—C6a—O1 is −95.6 (2)°. Although the synthesis started from enantiomerically pure *L*-serine, compound (I) crystallizes in a achiral space group ($P\bar{1}$): in the arbitrarily chosen asymmetric molecule, the configurations of the stereogenic centres are C3 *R*, C3A S, C6 *R*, and C6A *R*. This raecemization is in contrast to a related compound (Erdsack, Schürmann *et al.*, 2007).

Experimental

A small amount of the title compound which arose as a side product in the gold-catalyzed cyclization of α-hydroxyallenes (Erdsack & Krause, 2007) was suspended in a few drops of iso-hexane. Ethyl acetate was added dropwise until the compound was complete dissolved, and colourless blocks of (I) were obtained by slow evaporation at ambient temperature.

Refinement

The H atoms were placed in calculated positions, with C—H = 0.96–0.98 and N—H = 0.86 Å and refined as riding, with U_{iso}= 1.5U_{eq}; the methyl groups were allowed to rotate but not to tip. The –CF_3 fluorine atoms are disordered over two positions of equal occupancy.

Figures

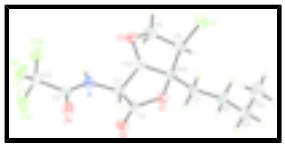

Fig. 1. : The molecular structure of (I) with displacement ellipsoids shown at the 20% probability level (arbitrary spheres for the H atoms). The F atoms are disordered over two positions; only one is shown.

rac-*N*-(6a-Butyl-6-chloro-2-oxoperhydrofuro[3,2-*b*]furan-3-yl)-2,2,2- trifluoroacetamide

Crystal data

$C_{12}H_{15}ClF_3NO_4$	Z = 2
M_r = 329.70	F_{000} = 340
Triclinic, $P\bar{1}$	D_x = 1.482 Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 7.674 (3) Å	Cell parameters from 8179 reflections
b = 9.586 (3) Å	θ = 3.1–25.3°

c = 11.590 (4) Å	μ = 0.31 mm^{-1}
α = 66.904 (13)º	T = 291 (1) K
β = 76.782 (14)º	Block, colourless
γ = 71.684 (13)º	0.10 × 0.08 × 0.08 mm
V = 739.1 (4) Å^3	

Data collection

Nonius KappaCCD area-detector diffractometer	2680 independent reflections
Radiation source: fine-focus sealed tube	959 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.031
Detector resolution: 19 vertical, 18 horizontal pixels mm^{-1}	θ_{max} = 25.3º
T = 291(1) K	θ_{min} = 3.1º
185 frames via ω–rotation (Δω = 2°) and two times 190 s per frame (four sets at different κ–angles) scans	$h = -9 \rightarrow 9$
Absorption correction: none	$k = -10 \rightarrow 11$
8179 measured reflections	$l = -13 \rightarrow 13$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.031	$w = [1.0 \exp(4.90(\sin\theta/\lambda)^2)]/[\sigma^2(F_o^2)]$
$wR(F^2)$ = 0.079	$(\Delta/\sigma)_{max} < 0.001$
S = 0.91	$\Delta\rho_{max}$ = 0.14 e Å^{-3}
2680 reflections	$\Delta\rho_{min}$ = −0.12 e Å^{-3}
219 parameters	Extinction correction: SHELXL97, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0297 (18)
Secondary atom site location: difference Fourier map	

Special details

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

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

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Cl	0.33628 (12)	0.95641 (10)	0.80355 (9)	0.0743 (3)	
O1	0.8738 (3)	0.7457 (2)	0.79610 (18)	0.0569 (6)	
C2	0.9876 (5)	0.7001 (4)	0.8845 (3)	0.0513 (8)	
O2	1.1278 (3)	0.5984 (2)	0.88767 (19)	0.0630 (6)	
C3	0.9078 (4)	0.7944 (3)	0.9721 (3)	0.0465 (8)	
H3	0.9723	0.8774	0.9464	0.070*	
C3A	0.7091 (4)	0.8701 (3)	0.9452 (3)	0.0500 (8)	
H3A	0.6688	0.9765	0.9480	0.075*	
O3	0.5884 (3)	0.7760 (2)	1.02971 (18)	0.0617 (6)	
C5	0.5403 (5)	0.6972 (4)	0.9643 (3)	0.0677 (10)	
H5A	0.4179	0.6799	0.9976	0.102*	
H5B	0.6284	0.5968	0.9727	0.102*	
C6	0.5449 (4)	0.8043 (3)	0.8274 (3)	0.0577 (9)	
H6	0.5670	0.7455	0.7705	0.087*	
C6A	0.7094 (4)	0.8714 (3)	0.8124 (3)	0.0494 (8)	
C7	0.7242 (4)	1.0219 (3)	0.7034 (3)	0.0583 (9)	
H7A	0.8377	1.0462	0.7033	0.087*	
H7B	0.6220	1.1064	0.7170	0.087*	
C8	0.7227 (5)	1.0161 (4)	0.5739 (3)	0.0705 (10)	
H8A	0.6093	0.9918	0.5736	0.106*	
H8B	0.8254	0.9322	0.5596	0.106*	
C9	0.7371 (6)	1.1697 (5)	0.4656 (3)	0.0884 (12)	
H9A	0.8433	1.1997	0.4716	0.133*	
H9B	0.7584	1.1522	0.3860	0.133*	
C10	0.5713 (7)	1.3005 (5)	0.4645 (4)	0.1211 (17)	
H10A	0.4630	1.2668	0.4709	0.182*	
H10B	0.5805	1.3870	0.3871	0.182*	
H10C	0.5627	1.3325	0.5348	0.182*	
N	0.9323 (3)	0.6989 (3)	1.1019 (2)	0.0534 (7)	
H0	0.8877	0.6180	1.1363	0.080*	
C11	1.0213 (4)	0.7313 (4)	1.1703 (3)	0.0548 (8)	
O4	1.0949 (3)	0.8376 (3)	1.13432 (19)	0.0769 (8)	
C12	1.0293 (8)	0.6182 (6)	1.3066 (4)	0.0761 (12)	
F1A	1.019 (3)	0.691 (2)	1.3743 (14)	0.142 (8)	0.50
F2A	0.896 (3)	0.543 (2)	1.347 (2)	0.131 (8)	0.50
F3A	1.189 (3)	0.5103 (18)	1.3085 (15)	0.152 (6)	0.50
F1B	0.950 (3)	0.6885 (19)	1.3945 (14)	0.125 (6)	0.50
F2B	0.950 (3)	0.509 (2)	1.3365 (19)	0.120 (7)	0.50
F3B	1.1950 (19)	0.557 (2)	1.3374 (14)	0.151 (7)	0.50

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl	0.0550 (6)	0.0754 (7)	0.0948 (7)	−0.0065 (5)	−0.0206 (5)	−0.0334 (5)

O1	0.0550 (15)	0.0568 (14)	0.0650 (15)	−0.0057 (12)	−0.0121 (12)	−0.0312 (11)
C2	0.051 (2)	0.044 (2)	0.058 (2)	−0.0196 (19)	−0.0050 (19)	−0.0110 (18)
O2	0.0540 (16)	0.0506 (14)	0.0762 (16)	−0.0040 (13)	−0.0103 (13)	−0.0193 (12)
C3	0.050 (2)	0.0396 (18)	0.051 (2)	−0.0147 (17)	−0.0094 (16)	−0.0127 (16)
C3A	0.056 (2)	0.0449 (18)	0.053 (2)	−0.0140 (18)	−0.0075 (17)	−0.0184 (15)
O3	0.0581 (16)	0.0673 (15)	0.0614 (14)	−0.0248 (13)	−0.0031 (11)	−0.0194 (12)
C5	0.062 (3)	0.058 (2)	0.087 (3)	−0.019 (2)	−0.014 (2)	−0.024 (2)
C6	0.048 (2)	0.053 (2)	0.080 (3)	−0.0040 (18)	−0.0157 (18)	−0.0339 (19)
C6A	0.046 (2)	0.0496 (19)	0.061 (2)	−0.0094 (17)	−0.0120 (16)	−0.0271 (17)
C7	0.067 (2)	0.053 (2)	0.058 (2)	−0.0166 (19)	−0.0177 (17)	−0.0156 (17)
C8	0.080 (3)	0.077 (3)	0.057 (2)	−0.014 (2)	−0.0190 (19)	−0.025 (2)
C9	0.104 (4)	0.095 (3)	0.060 (2)	−0.033 (3)	−0.016 (2)	−0.011 (2)
C10	0.142 (5)	0.083 (3)	0.115 (4)	−0.011 (3)	−0.049 (3)	−0.006 (3)
N	0.0655 (19)	0.0454 (16)	0.0494 (16)	−0.0208 (15)	−0.0139 (14)	−0.0074 (13)
C11	0.057 (2)	0.051 (2)	0.053 (2)	−0.0059 (18)	−0.0176 (17)	−0.0144 (17)
O4	0.097 (2)	0.0751 (17)	0.0720 (16)	−0.0455 (16)	−0.0281 (13)	−0.0117 (13)
C12	0.098 (5)	0.073 (3)	0.060 (3)	−0.028 (3)	−0.024 (3)	−0.013 (3)
F1A	0.28 (2)	0.159 (10)	0.036 (5)	−0.148 (12)	−0.003 (8)	−0.023 (5)
F2A	0.148 (9)	0.171 (17)	0.076 (6)	−0.108 (11)	−0.011 (5)	0.009 (9)
F3A	0.196 (13)	0.097 (6)	0.126 (9)	0.036 (6)	−0.103 (8)	−0.010 (5)
F1B	0.195 (11)	0.099 (7)	0.061 (6)	−0.032 (8)	0.015 (6)	−0.027 (5)
F2B	0.24 (2)	0.065 (4)	0.066 (7)	−0.070 (8)	−0.052 (10)	0.011 (4)
F3B	0.084 (7)	0.213 (16)	0.097 (7)	−0.010 (8)	−0.047 (5)	0.006 (8)

Geometric parameters (Å, °)

Cl—C6	1.784 (3)	C8—H8A	0.9700
O1—C2	1.350 (3)	C8—H8B	0.9700
O1—C6A	1.481 (3)	C9—C10	1.477 (5)
C2—O2	1.200 (3)	C9—H9A	0.9700
C2—C3	1.521 (4)	C9—H9B	0.9700
C3—N	1.441 (3)	C10—H10A	0.9600
C3—C3A	1.514 (4)	C10—H10B	0.9600
C3—H3	0.9800	C10—H10C	0.9600
C3A—O3	1.431 (3)	N—C11	1.329 (3)
C3A—C6A	1.534 (4)	N—H0	0.8600
C3A—H3A	0.9800	C11—O4	1.205 (3)
O3—C5	1.425 (3)	C11—C12	1.528 (5)
C5—C6	1.515 (4)	C12—F1A	1.213 (16)
C5—H5A	0.9700	C12—F2B	1.269 (16)
C5—H5B	0.9700	C12—F3B	1.290 (15)
C6—C6A	1.537 (4)	C12—F3A	1.328 (18)
C6—H6	0.9800	C12—F2A	1.332 (18)
C6A—C7	1.516 (4)	C12—F1B	1.364 (16)
C7—C8	1.526 (4)	F1A—F1B	0.53 (4)
C7—H7A	0.9700	F1A—F3B	1.65 (3)
C7—H7B	0.9700	F3A—F3B	0.67 (3)
C8—C9	1.532 (4)		
C2—O1—C6A	111.6 (2)	C10—C9—C8	113.9 (3)

O2—C2—O1	121.7 (3)	C10—C9—H9A	108.8
O2—C2—C3	128.7 (3)	C8—C9—H9A	108.8
O1—C2—C3	109.6 (3)	C10—C9—H9B	108.8
N—C3—C3A	115.4 (2)	C8—C9—H9B	108.8
N—C3—C2	111.9 (3)	H9A—C9—H9B	107.7
C3A—C3—C2	104.3 (2)	C9—C10—H10A	109.5
N—C3—H3	108.3	C9—C10—H10B	109.5
C3A—C3—H3	108.3	H10A—C10—H10B	109.5
C2—C3—H3	108.3	C9—C10—H10C	109.5
O3—C3A—C3	111.3 (2)	H10A—C10—H10C	109.5
O3—C3A—C6A	107.2 (2)	H10B—C10—H10C	109.5
C3—C3A—C6A	104.3 (2)	C11—N—C3	122.4 (2)
O3—C3A—H3A	111.2	C11—N—H0	118.8
C3—C3A—H3A	111.2	C3—N—H0	118.8
C6A—C3A—H3A	111.2	O4—C11—N	126.4 (3)
C5—O3—C3A	108.9 (2)	O4—C11—C12	119.1 (3)
O3—C5—C6	105.6 (2)	N—C11—C12	114.5 (3)
O3—C5—H5A	110.6	F1A—C12—F2B	123.9 (13)
C6—C5—H5A	110.6	F1A—C12—F3B	82.6 (12)
O3—C5—H5B	110.6	F2B—C12—F3B	108.5 (13)
C6—C5—H5B	110.6	F1A—C12—F3A	111.9 (13)
H5A—C5—H5B	108.8	F2B—C12—F3A	87.0 (13)
C5—C6—C6A	101.5 (2)	F3B—C12—F3A	29.8 (12)
C5—C6—Cl	110.3 (2)	F1A—C12—F2A	110.0 (14)
C6A—C6—Cl	110.6 (2)	F2B—C12—F2A	20.3 (18)
C5—C6—H6	111.3	F3B—C12—F2A	124.4 (14)
C6A—C6—H6	111.3	F3A—C12—F2A	106.7 (12)
Cl—C6—H6	111.3	F1A—C12—F1B	22.8 (16)
O1—C6A—C7	108.3 (2)	F2B—C12—F1B	104.4 (13)
O1—C6A—C3A	104.4 (2)	F3B—C12—F1B	100.4 (11)
C7—C6A—C3A	116.8 (2)	F3A—C12—F1B	126.9 (11)
O1—C6A—C6	104.2 (2)	F2A—C12—F1B	88.2 (13)
C7—C6A—C6	118.1 (3)	F1A—C12—C11	108.9 (9)
C3A—C6A—C6	103.5 (2)	F2B—C12—C11	115.1 (10)
C6A—C7—C8	114.2 (2)	F3B—C12—C11	113.4 (7)
C6A—C7—H7A	108.7	F3A—C12—C11	106.8 (9)
C8—C7—H7A	108.7	F2A—C12—C11	112.6 (11)
C6A—C7—H7B	108.7	F1B—C12—C11	113.8 (8)
C8—C7—H7B	108.7	F1B—F1A—C12	95 (3)
H7A—C7—H7B	107.6	F1B—F1A—F3B	131 (4)
C7—C8—C9	113.2 (3)	C12—F1A—F3B	50.7 (9)
C7—C8—H8A	108.9	F3B—F3A—C12	72 (3)
C9—C8—H8A	108.9	F1A—F1B—C12	62 (3)
C7—C8—H8B	108.9	F3A—F3B—C12	78 (3)
C9—C8—H8B	108.9	F3A—F3B—F1A	124 (3)
H8A—C8—H8B	107.8	C12—F3B—F1A	46.7 (8)
C6A—O1—C2—O2	179.4 (2)	O4—C11—C12—F3B	−53.6 (12)
C6A—O1—C2—C3	−0.1 (3)	N—C11—C12—F3B	125.6 (10)
O2—C2—C3—N	−39.3 (4)	O4—C11—C12—F3A	−84.7 (9)

O1—C2—C3—N	140.1 (2)	N—C11—C12—F3A	94.6 (9)
O2—C2—C3—C3A	−164.7 (3)	O4—C11—C12—F2A	158.6 (11)
O1—C2—C3—C3A	14.7 (3)	N—C11—C12—F2A	−22.1 (12)
N—C3—C3A—O3	−30.3 (3)	O4—C11—C12—F1B	60.2 (11)
C2—C3—C3A—O3	92.8 (2)	N—C11—C12—F1B	−120.5 (10)
N—C3—C3A—C6A	−145.6 (2)	F2B—C12—F1A—F1B	−34 (5)
C2—C3—C3A—C6A	−22.5 (3)	F3B—C12—F1A—F1B	−141 (4)
C3—C3A—O3—C5	−103.4 (3)	F3A—C12—F1A—F1B	−136 (4)
C6A—C3A—O3—C5	10.1 (3)	F2A—C12—F1A—F1B	−17 (4)
C3A—O3—C5—C6	−30.0 (3)	C11—C12—F1A—F1B	107 (4)
O3—C5—C6—C6A	36.8 (3)	F2B—C12—F1A—F3B	107.3 (16)
O3—C5—C6—Cl	−80.5 (2)	F3A—C12—F1A—F3B	5.6 (15)
C2—O1—C6A—C7	110.7 (2)	F2A—C12—F1A—F3B	124.0 (14)
C2—O1—C6A—C3A	−14.4 (3)	F1B—C12—F1A—F3B	141 (4)
C2—O1—C6A—C6	−122.7 (2)	C11—C12—F1A—F3B	−112.2 (9)
O3—C3A—C6A—O1	−95.6 (2)	F1A—C12—F3A—F3B	−11 (3)
C3—C3A—C6A—O1	22.6 (2)	F2B—C12—F3A—F3B	−137 (3)
O3—C3A—C6A—C7	144.8 (3)	F2A—C12—F3A—F3B	−132 (3)
C3—C3A—C6A—C7	−97.0 (3)	F1B—C12—F3A—F3B	−31 (3)
O3—C3A—C6A—C6	13.2 (3)	C11—C12—F3A—F3B	108 (2)
C3—C3A—C6A—C6	131.4 (2)	F3B—F1A—F1B—C12	−40 (3)
C5—C6—C6A—O1	79.4 (3)	F2B—C12—F1B—F1A	151 (4)
Cl—C6—C6A—O1	−163.56 (18)	F3B—C12—F1B—F1A	39 (4)
C5—C6—C6A—C7	−160.4 (3)	F3A—C12—F1B—F1A	54 (4)
Cl—C6—C6A—C7	−43.4 (3)	F2A—C12—F1B—F1A	164 (4)
C5—C6—C6A—C3A	−29.6 (3)	C11—C12—F1B—F1A	−82 (4)
Cl—C6—C6A—C3A	87.5 (3)	C12—F3A—F3B—F1A	9(2)
O1—C6A—C7—C8	62.9 (3)	F1A—C12—F3B—F3A	170 (3)
C3A—C6A—C7—C8	−179.7 (3)	F2B—C12—F3B—F3A	46 (3)
C6—C6A—C7—C8	−55.2 (4)	F2A—C12—F3B—F3A	60 (3)
C6A—C7—C8—C9	179.8 (3)	F1B—C12—F3B—F3A	155 (3)
C7—C8—C9—C10	−69.0 (4)	C11—C12—F3B—F3A	−83 (3)
C3A—C3—N—C11	−118.5 (3)	F2B—C12—F3B—F1A	−123.4 (13)
C2—C3—N—C11	122.5 (3)	F3A—C12—F3B—F1A	−170 (3)
C3—N—C11—O4	−2.0 (5)	F2A—C12—F3B—F1A	−109.2 (16)
C3—N—C11—C12	178.8 (4)	F1B—C12—F3B—F1A	−14.3 (14)
O4—C11—C12—F1A	36.3 (13)	C11—C12—F3B—F1A	107.4 (11)
N—C11—C12—F1A	−144.4 (12)	F1B—F1A—F3B—F3A	43 (6)
O4—C11—C12—F2B	−179.4 (12)	C12—F1A—F3B—F3A	−12 (3)
N—C11—C12—F2B	−0.1 (13)	F1B—F1A—F3B—C12	56 (5)

Fig. 1