Highly Stereoselective Additions of Tin Enolates to Nitroolefins and their Subsequent Conversion into Nitriles

*Barbara Mendler, Uli Kazmaier**

Institut für Organische Chemie, Universität des Saarlandes, D-66123 Saarbrücken, Germany.

E-mail: u.kazmaier@mx.uni-saarland.de

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2-(Trifluoroacetyl)amino-4-nitro-3-phenylbutyric acid *tert*-butylester (3a):

syn-Diastereomer: ^1H NMR (500 MHz): δ = 1.10 (s, 9 H, 6-H), 3.91 (ddd, $J_{7,12a}$ = 9.2 Hz, $J_{7,3}$ = 7.6 Hz, $J_{7,12b}$ = 6.3 Hz, 1 H, 7-H), 4.28 (dd, $J_{12b,12a}$ = 13.7 Hz, $J_{12b,7}$ = 6.3 Hz, 1 H, 12-H_b), 4.34 (dd, $J_{12a,12b}$ = 13.7 Hz, $J_{12a,7}$ = 9.2 Hz, 1 H, 12-H_a), 4.68 (dd, $J_{3,\text{N-H}}$ = $J_{3,7}$ = 7.6 Hz, 1 H, 3-H), 6.76 (d, $J_{\text{N-H},3}$ = 7.3 Hz, 1 H, N-H), 6.89–6.91, 7.02–7.03 (2 sh, 5 H, 9-H, 10-H, 11-H). ^{13}C NMR (125 MHz): δ = 27.7 (3 q, C-6), 46.1 (d, C-7), 55.0 (d, C-3), 76.6 (t, C-12), 85.0 (s, C-5), 115.4 (q, $J_{1,\text{F}}$ = 286.1 Hz, C-1), 128.3, 129.0, 129.2 (5 d, C-9, C-10, C-11), 133.7 (s, C-8), 156.9, (q, $J_{2,\text{F}}$ = 38.2 Hz, C-2), 167.3 (s, C-4).

anti-Diastereomer (selected signals): ^1H NMR (500 MHz): δ = 1.44 (s, 9 H, 6-H), 4.26 (ddd, $J_{7,12a}$ = 9.5 Hz, $J_{7,12b}$ = 6.6 Hz, $J_{7,3}$ = 3.8 Hz, 1 H, 7-H), 4.68 (dd, $J_{12a,12b}$ = 14.2 Hz, $J_{12a,7}$ = 9.5 Hz, 1 H, 12-H_a), 4.88 (dd, $J_{3,\text{N-H}}$ = $J_{3,7}$ = 7.2 Hz, 1 H, 3-H), 4.90 (dd, $J_{12b,12a}$ = 14.2 Hz, $J_{12b,7}$ = 6.6 Hz, 1 H, 12-H_b), 6.74 (d, $J_{\text{N-H},3}$ = 7.3 Hz, 1 H, N-H). ^{13}C NMR (125 MHz): δ = 27.9 (3 q, C-6), 46.0 (d, C-7), 54.5 (d, C-3), 76.2 (t, C-12), 85.0 (s, C-5), 128.1, 129.1, 129.2 (5 d, C-9, C-10, C-11), 133.1 (s, C-8), 167.0 (s, C-4).

Elemental analysis: C₁₆H₁₉F₃N₂O₅ (376.33) calcd.: C 51.07, H 5.09, N 7.44; found: C 51.00, H 5.84, N 7.46.

2-(Trifluoroacetyl)amino-3-nitromethyl-5-phenylpentoic acid *tert*-butylester (3b):

syn-Diastereomer: ^1H NMR (500 MHz): δ = 1.48 (s, 9 H, 6-H), 1.66 (m, 1 H, 8-H_a), 1.77 (m, 1 H, 8-H_b), 2.68–2.82 (sh, 2 H, 9-H), 4.36 (dd, $J_{14b,14a}$ = 12.9 Hz, $J_{14b,7}$ = 6.3 Hz, 1 H, 14-H_b), 4.45 (dd, $J_{14a,14b}$ = 12.9 Hz, $J_{14a,7}$ = 6.8 Hz, 1 H, 14-H_a), 4.74 (dd, $J_{3,\text{N-H}}$ = 7.6 Hz, $J_{3,7}$ = 3.2 Hz, 1 H, 3-H), 7.00 (d, $J_{\text{N-H},3}$ = 7.3 Hz, 1 H, N-H), 7.11–7.29 (sh, 5 H, 11-H, 12-H, 13-H). ^{13}C NMR (125 MHz): δ = 27.9 (3 q, C-6), 30.8 (t, C-8), 32.7 (t, C-9), 39.1 (d, C-7), 53.5 (d, C-3), 76.1 (t, C-14), 85.0 (s, C-5), 115.5 (q, $J_{1,\text{F}}$ = 286.1 Hz, C-1), 126.5 (d, C-13), 128.3, 128.7 (4 d, C-11, C-12), 139.9 (s, C-10), 157.4 (q, $J_{2,\text{F}}$ = 38.1 Hz, C-2), 168.0 (s, C-4).

anti-Diastereomer (selected signals): ^1H NMR (500 MHz): δ = 2.97 (m, 1 H, 9-H), 4.33 (dd, $J_{14b,14a}$ = 14.0 Hz, $J_{14b,7}$ = 5.9 Hz, 1 H, 14-H_b), 4.50 (dd, $J_{14a,14b}$ = 14.0 Hz, $J_{14a,7}$ = 7.8 Hz, 1 H, 14-H_a). ^{13}C NMR (125 MHz): δ = 29.9 (t, C-8), 32.8 (t, C-9), 39.4 (d, C-7), 54.1 (d, C-3), 126.6 (d, C-13), 128.3, 128.8 (4 d, C-11, C-12), 140.0 (s, C-10), 168.1 (s, C-4).

Elemental analysis: C₁₈H₂₃F₃N₂O₅ (404.39) calcd.: C 53.46, H 5.73, N 6.93; found: C 53.35, H 5.82, N 6.75.

2-(Trifluoroacetyl)amino-4-methyl-3-nitromethylpentanoic acid *tert*-butylester (3c):

syn-Diastereomer: ^1H NMR (500 MHz): δ = 0.62, 0.76 (2 d, $J_{9,8}$ = 6.9 Hz, 6 H, 9-H), 1.33 (s, 9 H, 6-H), 1.53 (dsept, $J_{8,7} = J_{8,9}$ = 6.8 Hz, 1 H, 8-H), 2.65 (dddd, $J_{7,10a} = 7.3$ Hz, $J_{7,8} = 6.8$ Hz, $J_{7,10b} = 5.1$ Hz, $J_{7,3} = 4.4$ Hz, 1 H, 7-H), 3.86 (dd, $J_{10b,10a} = 13.6$ Hz, $J_{10b,7} = 5.1$ Hz, 1 H, 10-H_b), 3.90 (dd, $J_{10a,10b} = 13.6$ Hz, $J_{10a,7} = 7.3$ Hz, 1 H, 10-H_a), 4.83 (dd, $J_{3,\text{N-H}} = 8.8$ Hz, $J_{3,7} = 4.4$ Hz, 1 H, 3-H), 7.28 (d, $J_{\text{N-H},3} = 8.4$ Hz, 1 H, N-H). ^{13}C NMR (125 MHz): δ = 18.8, 20.7 (2 q, C-9), 28.1 (3 q, C-6), 28.4 (d, C-8), 45.5 (d, C-7), 53.4 (d, C-3), 74.3 (t, C-10), 84.6 (s, C-5), 115.6 (q, $J_{1,\text{F}} = 286.1$ Hz, C-1), 157.5 (q, $J_{2,\text{F}} = 38.1$ Hz, C-2), 168.6 (s, C-4).

anti-Diastereomer (selected signals): ^1H NMR (500 MHz): δ = 0.58 (d, $J_{9,8}$ = 6.8 Hz, 6 H, 9-H), 1.30 (s, 9 H, 6-H), 2.55 (dddd, $J_{7,10a} = 7.6$ Hz, $J_{7,8} = 6.3$ Hz, $J_{7,3} = 5.4$ Hz, $J_{7,10b} = 4.3$ Hz, 1 H, 7-H), 3.89 (dd, $J_{10b,10a} = 14.7$ Hz, $J_{10b,7} = 4.3$ Hz, 1 H, 7-H), 4.25 (dd, $J_{10a,10b} = 14.7$ Hz, $J_{10a,7} = 7.6$ Hz, 1 H, 11-H_a), 4.60 (dd, $J_{3,\text{N-H}} = 7.6$ Hz, $J_{3,7} = 5.4$ Hz, 1 H, 3-H), 7.06 (d, $J_{\text{N-H},3} = 6.3$ Hz, 1 H, N-H). ^{13}C NMR (125 MHz): δ = 19.1, 21.2 (2 q, C-9, C-10), 54.0 (d, C-3), 84.9 (s, C-5), 168.3 (s, C-4).

Elemental analysis: $\text{C}_{13}\text{H}_{21}\text{F}_3\text{N}_2\text{O}_5$ (342.33) calcd.: C 45.61, H 6.18, N 8.18; found: C 45.80, H 6.32, N 8.16.

2-(Trifluoroacetyl)amino-4,4-dimethyl-3-nitromethylpentanoic acid *tert*-butylester (3d):

syn-Diastereomer: ^1H NMR (500 MHz): δ = 1.01 (s, 9 H, 9-H), 1.44 (s, 9 H, 6-H), 2.87 (ddd, $J_{7,10a} = 9.8$ Hz, $J_{7,10b} = 4.1$ Hz, $J_{7,3} = 1.6$ Hz, 1 H, 7-H), 4.41 (dd, $J_{10a,10b} = 12.7$ Hz, $J_{10a,7} = 9.8$ Hz, 1 H, 10-H_a), 4.56 (dd, $J_{10b,10a} = 12.7$ Hz, $J_{10b,7} = 4.1$ Hz, 1 H, 10-H_b), 4.98 (dd, $J_{3,\text{N-H}} = 9.8$ Hz, $J_{3,7} = 1.3$ Hz, 1 H, 3-H), 7.06 (d, $J_{\text{N-H},3} = 9.5$ Hz, 1 H, N-H). ^{13}C NMR (125 MHz): δ = 27.6, 27.6 (6 q, C-6, C-9), 33.8 (s, C-8), 48.7 (d, C-7), 51.1 (d, C-3), 73.7 (t, C-10), 84.4 (s, C-5), 115.6 (q, $J_{1,\text{F}} = 286.1$ Hz, C-1), 157.5 (q, $J_{2,\text{F}} = 38.1$ Hz, C-2), 168.7 (s, C-4).

anti-Diastereomer (selected signals): ^1H NMR (500 MHz): 1.04 (s, 9 H, 9-H), 1.46 (s, 9 H, 6-H), 2.59 (ddd, $J_{7,10a} = 6.0$ Hz, $J_{7,10b} = 3.5$ Hz, $J_{7,3} = 2.6$ Hz, 1 H, 7-H), 4.50 (dd, $J_{10b,10a} = 14.9$ Hz, $J_{10b,7} = 3.5$ Hz, 1 H, 10-H_b), 4.78 (dd, $J_{3,\text{N-H}} = 9.1$ Hz, $J_{3,7} = 2.3$ Hz, 1 H, 3-H), 4.79 (dd, $J_{10a,10b} = 15.2$ Hz, $J_{10a,7} = 5.9$ Hz, 1 H, 10-H_a). ^{13}C NMR (125 MHz): δ = 50.1 (d, C-7), 52.9 (d, C-3), 84.7 (s, C-5).

Elemental analysis: $\text{C}_{14}\text{H}_{23}\text{F}_3\text{N}_2\text{O}_5$ (356.34) calcd.: C 47.19, H 6.51, N 7.86; found: C 47.28, H 6.28, N 7.71.

2-(Trifluoroacetyl)amino-3-(2-methoxyphenyl)-4-nitrobutyric acid *tert*-butylester (3e):

syn-Diastereomer: ^1H NMR (500 MHz): δ = 1.20 (s, 9 H, 6-H), 3.87 (s, 3 H, 14-H), 4.16 (ddd, $J_{7,15a}$ = 8.5 Hz, $J_{7,3}$ = 8.2 Hz, $J_{7,15b}$ = 6.0 Hz, 1 H, 7-H), 4.79 (dd, $J_{15b,15a}$ = 13.6 Hz, $J_{15b,7}$ = 6.0 Hz, 1 H, 15-H_b), 4.95 (dd, $J_{15a,15b}$ = 13.6 Hz, $J_{15a,7}$ = 8.5 Hz, 1 H, 15-H_a), 4.98 (dd, $J_{3,7}$ = $J_{3,\text{N-H}}$ = 8.2 Hz, 1 H, 3-H), 6.89–6.92 (sh, 2 H, 10-H, 12-H), 7.04 (dd, $J_{9,10}$ = 7.3 Hz, $J_{9,11}$ = 1.3 Hz, 1 H, 9-H), 7.23 (d, $J_{\text{N-H},3}$ = 7.6 Hz, 1 H, N-H), 7.30 (td, $J_{10,9}$ = $J_{10,11}$ = 7.6 Hz, $J_{10,12}$ = 1.5 Hz, 1 H, 10-H). ^{13}C NMR (125 MHz): δ = 27.6 (3 q, C-6), 42.8 (d, C-7), 54.3 (d, C-3), 55.5 (q, C-14), 75.8 (t, C-15), 83.9 (s, C-5), 111.2 (d, C-12), 115.6 (q, $J_{1,\text{F}}$ = 286.1 Hz, C-1), 121.1 (d, C-10), 122.3 (s, C-8), 130.1, 130.2 (2 d, C-9, C-11), 157.0 (q, $J_{2,\text{F}}$ = 38.1 Hz, C-2), 157.5 (s, C-13), 167.7 (s, C-4).

anti-Diastereomer: ^1H NMR (500 MHz): δ = 1.24 (s, 9 H, 6-H), 3.28 (s, 3 H, 14-H), 4.28 (dt, $J_{7,15a}$ = 8.5 Hz, $J_{7,3}$ = $J_{7,15b}$ = 6.3 Hz, 1 H, 7-H), 4.50 (dd, $J_{15b,15a}$ = 13.6 Hz, $J_{15b,7}$ = 6.3 Hz, 1 H, 15-H_b), 4.57 (dd, $J_{15a,15b}$ = 13.6 Hz, $J_{15a,7}$ = 8.5 Hz, 1 H, 15-H_a), 4.95 (dd, $J_{3,\text{N-H}}$ = 8.4 Hz, $J_{3,7}$ = 6.3 Hz, 1 H, 3-H), 7.56 (d, $J_{\text{N-H},3}$ = 8.2 Hz, 1 H, N-H). ^{13}C NMR (125 MHz): δ = 27.7 (3 q, C-6), 43.6 (d, C-7), 54.6 (d, C-3), 55.5 (q, C-14), 75.4 (t, C-15), 83.9 (s, C-5), 111.6 (d, C-12), 115.7 (q, $J_{1,\text{F}}$ = 286.1 Hz, C-1), 121.5 (d, C-10), 121.9 (s, C-8), 130.5, 132.2 (2 d, C-9, C-11), 157.0 (s, C-13), 157.1 (q, $J_{2,\text{F}}$ = 37.2 Hz, C-2), 167.0 (s, C-4).

Elemental analysis: $\text{C}_{17}\text{H}_{21}\text{F}_3\text{N}_2\text{O}_6$ (406.36) calcd.: C 50.25, H 5.21, N 6.89; found: C 50.22, H 5.21, N 6.74.

2-(Trifluoroacetyl)amino-3-nitromethyl-4-phenylpentanoic acid *tert*-butylester (3f):

syn,syn-Diastereomer: ^1H NMR (500 MHz): δ = 0.90 (d, $J_{9,8}$ = 7.3 Hz, 3 H, 9-H), 1.28 (s, 9 H, 6-H), 2.68 (dq, $J_{8,7}$ = 10.1 Hz, $J_{8,9}$ = 7.2 Hz, 1 H, 8-H), 3.22 (dddd, $J_{7,8}$ = 10.4 Hz, $J_{7,14a}$ = 7.9 Hz, $J_{7,14b}$ = 5.4 Hz, $J_{7,3}$ = 2.9 Hz, 1 H, 7-H), 3.95 (dd, $J_{14a,14b}$ = 13.6 Hz, $J_{14a,7}$ = 7.6 Hz, 1 H, 14-H_a), 4.05 (dd, $J_{14b,14a}$ = 13.6 Hz, $J_{14b,7}$ = 5.4 Hz, 1 H, 14-H_b), 4.56 (dd, $J_{3,\text{N-H}}$ = 8.2 Hz, $J_{3,7}$ = 2.8 Hz, 1 H, 3-H), 6.82 (bs, 1 H, N-H), 7.10–7.22 (sh, 5 H, 11-H, 12-H, 13-H). ^{13}C NMR (125 MHz): δ = 19.2 (q, C-9), 27.8 (3 q, C-6), 40.0 (d, C-8), 45.3 (d, C-7), 53.8 (d, C-3), 75.0 (t, C-14), 84.6 (s, C-5), 115.4 (q, $J_{1,\text{F}}$ = 286.1 Hz, C-1), 127.4, 127.6, 129.1 (5 d, C-11, C-12, C-13), 142.8 (s, C-10), 157.0 (q, $J_{2,\text{F}}$ = 37.2 Hz, C-2), 168.0 (s, C-4).

Elemental analysis: $\text{C}_{18}\text{H}_{23}\text{F}_3\text{N}_2\text{O}_5$ (404.39) calcd.: C 53.46, H 5.73, N 6.93; found: C 53.35, H 5.42, N 6.86.

2-(Trifluoroacetyl)amino-3-cyano-4-methylpentanoic acid *tert*-butylester (4c):

syn-Diastereomer: ^1H NMR (500 MHz): δ = 1.11, 1.16 (2 d, $J_{9,8}$ = 6.6 Hz, 6 H, 9-H), 1.51 (s, 9 H, 6-H), 1.86 (dsept, $J_{8,7}$ = 8.8 Hz, $J_{8,9}$ = 6.6 Hz, 1 H, 8-H), 2.94 (dd, $J_{7,8}$ = 8.9 Hz, $J_{7,3}$ = 3.8 Hz, 1 H, 7-H), 4.83 (dd, $J_{3,\text{N-H}}$ = 9.2 Hz, $J_{3,7}$ = 3.8 Hz, 1 H, 3-H), 6.87 (d, $J_{\text{N-H},3}$ = 7.6 Hz, 1 H, N-H). ^{13}C NMR (125 MHz): δ = 20.6, 20.6 (2 q, C-9), 27.8 (3 q, C-6), 28.2 (d, C-8), 42.9 (d, C-7), 51.7 (d, C-3), 85.3 (s, C-5), 115.5 (q, $J_{1,\text{F}}$ = 282.3 Hz, C-1), 117.1 (s, C-10), 157.5 (q, $J_{2,\text{F}}$ = 38.2 Hz, C-2), 166.8 (s, C-4).

Elemental analysis: $\text{C}_{13}\text{H}_{19}\text{F}_3\text{N}_2\text{O}_3$ (308.30) calcd.: C 50.65, H 6.21, N 9.09; found: C 50.64, H 6.23, N 9.10.

2-(Trifluoroacetyl)amino-3-cyano-4-phenylpentanoic acid *tert*-butylester (4f):

syn,syn-Diastereomer: ^1H NMR (500 MHz): δ = 1.48 (s, 9 H, 6-H), 1.50 (d, $J_{9,8}$ = 7.3 Hz, 3 H, 9-H), 2.98 (dq, $J_{8,7}$ = 10.4 Hz, $J_{8,9}$ = 7.0 Hz, 1 H, 8-H), 3.50 (dd, $J_{7,8}$ = 10.4 Hz, $J_{7,3}$ = 2.9 Hz, 1 H, 7-H), 4.49 (dd, $J_{3,\text{N-H}}$ = 9.2 Hz, $J_{3,7}$ = 2.9 Hz, 1 H, 3-H), 6.79 (bs, 1 H, N-H), 7.16 (d, $J_{11,12}$ = 7.3 Hz, 2 H, 11-H), 7.28 (t, $J_{13,12}$ = 7.3 Hz, 1 H, 13-H), 7.35 (t, $J_{12,11}$ = $J_{12,13}$ = 7.3 Hz, 2 H, 12-H). ^{13}C NMR (125 MHz): δ = 21.1 (q, C-9), 27.8 (3 q, C-6), 39.5 (d, C-8), 41.9 (d, C-7), 52.2 (d, C-3), 85.1 (s, C-5), 115.4 (q, $J_{1,\text{F}}$ = 286.1 Hz, C-1), 117.3 (s, C-14), 127.1 (2 d, C-11), 128.0 (C-13), 129.2 (2 d, C-12), 140.7 (s, C-10), 157.1 (q, $J_{2,\text{F}}$ = 38.2 Hz, C-2), 166.4 (s, C-4).

Elemental analysis: $\text{C}_{18}\text{H}_{21}\text{F}_3\text{N}_2\text{O}_3$ (370.37) calcd.: C 58.53, H 5.46, N 7.58; found: C 58.62, H 5.39, N 7.39.

2-(Trifluoroacetyl)amino-4-nitro-3-phenylbutyric acid *tert*-butylester (3a)

Table 1. Crystal data and structure refinement for **3a**.

Identification code	sh1925	
Empirical formula	C ₁₆ H ₁₈ F ₃ N ₂ O ₅	
Formula weight	375.32	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 16.089(3) Å	$\alpha = 90^\circ$.
	b = 5.6320(10) Å	$\beta = 108.29(3)^\circ$.
	c = 21.119(4) Å	$\gamma = 90^\circ$.
Volume	1817.0(6) Å ³	
Z	4	
Density (calculated)	1.372 Mg/m ³	
Absorption coefficient	0.121 mm ⁻¹	
F(000)	780	
Crystal size	0.35 x 0.31 x 0.15 mm ³	
Theta range for data collection	1.91 to 29.28°.	
Index ranges	-22 ≤ h ≤ 20, 0 ≤ k ≤ 7, 0 ≤ l ≤ 28	
Reflections collected	4923	
Independent reflections	4923 [R(int) = 0.0000]	
Completeness to theta = 29.28°	99.1 %	
Absorption correction	N/A	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	4923 / 0 / 235	
Goodness-of-fit on F ²	1.609	
Final R indices [I > 2σ(I)]	R1 = 0.1500, wR2 = 0.2565	
R indices (all data)	R1 = 0.2957, wR2 = 0.3063	
Largest diff. peak and hole	0.532 and -0.467 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **3a**. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	$U(\text{eq})$
O(1)	6024(2)	403(6)	2425(2)	67(1)
O(2)	5936(3)	3572(9)	3043(2)	92(1)
O(3)	4041(4)	-633(14)	4454(3)	147(3)
O(4)	7228(5)	-3269(15)	4372(3)	148(3)
O(5)	4058(4)	-4333(13)	4391(3)	165(3)
N(1)	6724(3)	514(12)	4091(2)	97(2)
N(2)	4350(4)	-2430(17)	4334(3)	100(2)
C(1)	5141(3)	-331(9)	3663(2)	65(1)
C(2)	5147(4)	-2352(11)	4130(3)	81(2)
C(3)	6021(3)	-289(11)	3515(2)	68(2)
C(4)	5992(3)	1466(13)	2975(3)	69(2)
C(5)	5968(4)	1713(10)	1800(2)	67(2)
C(6)	6730(4)	3356(12)	1924(3)	102(2)
C(7)	5096(4)	2967(12)	1559(3)	95(2)
C(8)	6030(5)	-230(11)	1337(3)	116(3)
C(9)	7252(6)	-1170(20)	4430(4)	116(3)
C(10)	8043(6)	30(20)	5005(5)	137(3)
C(11)	4377(3)	-420(10)	3020(2)	59(1)
C(12)	4275(4)	-2307(10)	2594(3)	72(2)
C(13)	3597(4)	-2357(11)	1990(3)	80(2)
C(14)	3033(4)	-514(12)	1815(3)	77(2)
C(15)	3108(4)	1343(11)	2235(3)	78(2)
C(16)	3773(4)	1385(10)	2830(3)	71(2)
F(1A)	8694(5)	446(18)	4780(4)	124(2)
F(2A)	8420(14)	-2950(50)	5255(11)	155(8)
F(3A)	7849(9)	-950(30)	5548(6)	137(4)
F(2B)	7889(7)	2380(20)	5167(6)	120(3)
F(1B)	8327(11)	2140(30)	4870(7)	127(5)
F(3B)	7892(7)	820(30)	5482(6)	124(4)
F(1C)	8720(8)	-1370(30)	5011(7)	126(4)
F(3C)	8456(10)	-1360(30)	5458(7)	126(4)

Table 3. Bond lengths [Å] and angles [°] for **3a**.

O(1)-C(4)	1.321(6)	O(1)-C(4)-C(3)	111.7(5)	F(3C)-F(2A)-F(1C)	62.6(17)
O(1)-C(5)	1.490(5)	O(1)-C(5)-C(8)	102.7(4)	F(3C)-F(2A)-F(3A)	36.8(14)
O(2)-C(4)	1.201(6)	O(1)-C(5)-C(6)	109.5(4)	F(1C)-F(2A)-F(3A)	90.1(17)
O(3)-N(2)	1.189(7)	C(8)-C(5)-C(6)	110.5(5)	F(3C)-F(2A)-C(10)	41.6(13)
O(4)-C(9)	1.186(10)	O(1)-C(5)-C(7)	108.8(4)	F(1C)-F(2A)-C(10)	47.9(11)
O(5)-N(2)	1.192(7)	C(8)-C(5)-C(7)	111.6(5)	F(3A)-F(2A)-C(10)	46.9(8)
N(1)-C(9)	1.325(11)	C(6)-C(5)-C(7)	113.2(5)	F(3B)-F(3A)-F(3C)	94.7(17)
N(1)-C(3)	1.449(6)	O(4)-C(9)-N(1)	131.6(10)	F(3B)-F(3A)-C(10)	56.8(10)
N(2)-C(2)	1.475(8)	O(4)-C(9)-C(10)	119.4(10)	F(3C)-F(3A)-C(10)	59.3(10)
C(1)-C(2)	1.506(7)	N(1)-C(9)-C(10)	109.0(9)	F(3B)-F(3A)-F(2A)	122.4(17)
C(1)-C(11)	1.519(6)	F(3B)-C(10)-F(3C)	77.8(12)	F(3C)-F(3A)-F(2A)	33.2(12)
C(1)-C(3)	1.542(7)	F(3B)-C(10)-F(1A)	130.1(11)	C(10)-F(3A)-F(2A)	71.0(11)
C(3)-C(4)	1.499(7)	F(3C)-C(10)-F(1A)	95.6(11)	F(3B)-F(2B)-F(1B)	111.4(15)
C(5)-C(8)	1.491(7)	F(3B)-C(10)-F(1B)	91.4(12)	F(3B)-F(2B)-C(10)	55.2(9)
C(5)-C(6)	1.492(8)	F(3C)-C(10)-F(1B)	125.9(13)	F(1B)-F(2B)-C(10)	62.9(11)
C(5)-C(7)	1.509(7)	F(1A)-C(10)-F(1B)	52.7(8)	F(2B)-F(1B)-F(1A)	130.5(17)
C(9)-C(10)	1.609(12)	F(3B)-C(10)-F(1C)	126.2(12)	F(2B)-F(1B)-C(10)	70.3(12)
C(10)-F(3B)	1.193(13)	F(3C)-C(10)-F(1C)	52.5(9)	F(1A)-F(1B)-C(10)	62.2(10)
C(10)-F(3C)	1.255(14)	F(1A)-C(10)-F(1C)	50.5(8)	F(3A)-F(3B)-F(2B)	152.0(17)
C(10)-F(1A)	1.298(11)	F(1B)-C(10)-F(1C)	101.2(12)	F(3A)-F(3B)-C(10)	78.1(12)
C(10)-F(1B)	1.330(16)	F(3B)-C(10)-F(3A)	45.2(8)	F(2B)-F(3B)-C(10)	75.6(11)
C(10)-F(1C)	1.342(15)	F(3C)-C(10)-F(3A)	47.6(8)	F(3A)-F(3B)-F(3C)	44.3(10)
C(10)-F(3A)	1.396(15)	F(1A)-C(10)-F(3A)	141.9(11)	F(2B)-F(3B)-F(3C)	120.7(13)
C(10)-F(2B)	1.407(14)	F(1B)-C(10)-F(3A)	135.1(12)	C(10)-F(3B)-F(3C)	52.9(8)
C(10)-F(2A)	1.810(3)	F(1C)-C(10)-F(3A)	98.6(11)	F(1A)-F(1C)-F(3C)	112.2(16)
C(11)-C(12)	1.369(7)	F(3B)-C(10)-F(2B)	49.2(8)	F(1A)-F(1C)-F(2A)	152.9(18)
C(11)-C(16)	1.376(7)	F(3C)-C(10)-F(2B)	119.6(12)	F(3C)-F(1C)-F(2A)	49.4(12)
C(12)-C(13)	1.395(7)	F(1A)-C(10)-F(2B)	98.4(9)	F(1A)-F(1C)-C(10)	62.7(9)
C(13)-C(14)	1.352(7)	F(1B)-C(10)-F(2B)	46.8(8)	F(3C)-F(1C)-C(10)	59.9(10)
C(14)-C(15)	1.351(7)	F(1C)-C(10)-F(2B)	139.1(11)	F(2A)-F(1C)-C(10)	90.4(15)
C(15)-C(16)	1.371(7)	F(3A)-C(10)-F(2B)	93.9(10)	F(2A)-F(3C)-F(3A)	110.0(2)
F(1A)-F(1C)	1.128(14)	F(3B)-C(10)-C(9)	118.1(10)	F(2A)-F(3C)-F(1C)	68.0(17)
F(1A)-F(1B)	1.166(16)	F(3C)-C(10)-C(9)	114.5(11)	F(3A)-F(3C)-F(1C)	137.3(17)
F(2A)-F(3C)	0.980(2)	F(1A)-C(10)-C(9)	109.7(8)	F(2A)-F(3C)-C(10)	106.9(19)
F(2A)-F(1C)	1.200(2)	F(1B)-C(10)-C(9)	117.2(11)	F(3A)-F(3C)-C(10)	73.0(13)
F(2A)-F(3A)	1.690(3)	F(1C)-C(10)-C(9)	101.8(9)	F(1C)-F(3C)-C(10)	67.6(11)
F(3A)-F(3B)	1.011(15)	F(3A)-C(10)-C(9)	97.1(9)	F(2A)-F(3C)-F(3B)	142.0(2)
F(3A)-F(3C)	1.078(15)	F(2B)-C(10)-C(9)	115.0(10)	F(3A)-F(3C)-F(3B)	40.9(10)
F(2B)-F(3B)	1.100(14)	F(3B)-C(10)-F(2A)	103.7(13)	F(1C)-F(3C)-F(3B)	113.8(16)
F(2B)-F(1B)	1.089(16)	F(3C)-C(10)-F(2A)	31.4(9)	C(10)-F(3C)-F(3B)	49.3(8)
F(3B)-F(3C)	1.540(2)	F(1A)-C(10)-F(2A)	92.2(10)		
F(1C)-F(3C)	1.151(16)	F(1B)-C(10)-F(2A)	141.5(13)		
		F(1C)-C(10)-F(2A)	41.7(9)		
C(4)-O(1)-C(5)	123.0(4)	F(3A)-C(10)-F(2A)	62.2(11)		
C(9)-N(1)-C(3)	115.4(7)	F(2B)-C(10)-F(2A)	150.5(12)		
O(3)-N(2)-O(5)	122.6(7)	C(9)-C(10)-F(2A)	86.6(9)		
O(3)-N(2)-C(2)	119.8(7)	C(12)-C(11)-C(16)	117.0(5)		
O(5)-N(2)-C(2)	117.5(8)	C(12)-C(11)-C(1)	120.6(5)		
C(2)-C(1)-C(11)	113.4(5)	C(16)-C(11)-C(1)	122.4(5)		
C(2)-C(1)-C(3)	109.1(4)	C(11)-C(12)-C(13)	121.0(5)		
C(11)-C(1)-C(3)	110.9(4)	C(14)-C(13)-C(12)	120.0(6)		
N(2)-C(2)-C(1)	112.8(5)	C(15)-C(14)-C(13)	120.1(5)		
N(1)-C(3)-C(4)	105.3(5)	C(14)-C(15)-C(16)	119.9(6)		
N(1)-C(3)-C(1)	111.0(4)	C(15)-C(16)-C(11)	122.1(5)		
C(4)-C(3)-C(1)	110.6(4)	F(1C)-F(1A)-F(1B)	128.4(13)		
O(2)-C(4)-O(1)	125.3(6)	F(1C)-F(1A)-C(10)	66.7(9)		
O(2)-C(4)-C(3)	123.0(5)	F(1B)-F(1A)-C(10)	65.1(9)		

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **3a**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	82(2)	69(2)	55(2)	2(2)	29(2)	4(2)
O(2)	115(3)	90(3)	69(3)	-10(3)	27(2)	4(3)
O(3)	141(5)	186(6)	158(5)	-32(5)	110(4)	-12(5)
O(4)	112(5)	225(7)	101(4)	73(6)	24(3)	60(6)
O(5)	141(5)	158(6)	206(6)	36(5)	70(4)	-45(4)
N(1)	56(3)	182(6)	44(2)	23(3)	2(2)	22(3)
N(2)	101(5)	135(6)	75(3)	8(4)	42(3)	-26(5)
C(1)	71(3)	65(4)	61(3)	-7(3)	26(3)	7(3)
C(2)	97(4)	94(4)	61(3)	0(3)	37(3)	4(4)
C(3)	58(3)	94(4)	54(3)	11(3)	21(2)	17(3)
C(4)	60(3)	83(4)	66(4)	-7(4)	23(3)	3(3)
C(5)	84(4)	66(4)	53(3)	9(3)	24(3)	5(3)
C(6)	99(5)	108(5)	113(5)	29(4)	51(4)	-6(4)
C(7)	88(4)	120(5)	71(4)	22(4)	16(3)	9(4)
C(8)	207(8)	89(5)	72(4)	-1(4)	72(5)	8(5)
C(9)	83(6)	207(10)	64(4)	11(7)	30(4)	0(8)
C(11)	63(3)	59(3)	60(3)	-2(3)	27(3)	2(3)
C(12)	85(4)	67(4)	67(3)	-1(3)	27(3)	14(3)
C(13)	98(4)	77(4)	62(3)	-11(3)	22(3)	10(4)
C(14)	68(4)	90(5)	68(4)	2(4)	16(3)	3(4)
C(15)	60(4)	72(4)	99(4)	3(4)	23(3)	8(3)
C(16)	70(4)	57(3)	91(4)	-9(3)	33(3)	0(3)

2-(Trifluoroacetyl)amino-3-nitromethyl-4-phenylpentanoic acid *tert*-butylester (3f)

Table 1. Crystal data and structure refinement for **3f**.

Identification code	shelxs1965	
Empirical formula	C ₁₈ H ₂₂ F ₃ N ₂ O ₅	
Formula weight	403.38	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 40.210(8) Å	α = 90°.
	b = 10.401(2) Å	β = 98.72(3)°.
	c = 20.455(4) Å	γ = 90°.
Volume	8456(3) Å ³	
Z	16	
Density (calculated)	1.267 Mg/m ³	
Absorption coefficient	0.109 mm ⁻¹	
F(000)	3376	
Crystal size	0.38 x 0.23 x 0.1 mm ³	
Theta range for data collection	2.01 to 24.41°.	
Index ranges	-46 ≤ h ≤ 45, -11 ≤ k ≤ 10, -23 ≤ l ≤ 22	
Reflections collected	25898	
Independent reflections	6392 [R(int) = 0.1131]	
Completeness to theta = 24.41°	91.8 %	
Absorption correction	N/A	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	6392 / 0 / 505	
Goodness-of-fit on F ²	0.947	
Final R indices [I > 2σ(I)]	R1 = 0.0678, wR2 = 0.1592	
R indices (all data)	R1 = 0.1542, wR2 = 0.1876	
Largest diff. peak and hole	0.612 and -0.303 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **3f**. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)					
O(1)	1707(1)	1457(3)	3731(2)	74(1)	C(18)	1914(1)	6312(5)	2816(3)	83(2)
O(2)	1246(1)	1107(3)	4210(2)	75(1)	C(19)	621(1)	9421(4)	322(2)	54(1)
O(3)	997(1)	4666(5)	3187(2)	145(2)	C(20)	713(1)	8119(5)	626(2)	54(1)
O(4)	2138(2)	2295(8)	5526(3)	231(4)	C(21)	617(1)	6745(6)	1570(3)	79(2)
O(5)	1904(2)	2810(9)	6287(3)	259(5)	C(22)	393(2)	7011(7)	2087(3)	131(3)
O(6)	902(1)	7381(3)	419(1)	68(1)	C(23)	981(2)	6653(7)	1856(3)	125(2)
O(7)	558(1)	7912(3)	1143(1)	66(1)	C(24)	496(2)	5593(7)	1172(4)	129(2)
O(8)	29(1)	8797(4)	-534(2)	89(1)	C(25)	291(1)	9017(5)	-752(2)	72(2)
O(9)	1184(1)	12182(5)	-319(2)	144(2)	C(26)	295(2)	9009(8)	-1486(3)	97(2)
O(10)	1054(1)	13713(5)	295(3)	133(2)	C(27)	887(1)	10464(4)	547(2)	55(1)
N(1)	1112(1)	3715(4)	4186(2)	59(1)	C(28)	757(1)	11777(5)	291(2)	70(1)
N(2)	1912(2)	2792(7)	5737(3)	132(2)	C(29)	1011(1)	10471(5)	1298(2)	58(1)
N(3)	587(1)	9315(4)	-397(2)	63(1)	C(30)	729(1)	10782(5)	1709(2)	85(2)
N(4)	1025(1)	12623(6)	73(3)	89(1)	C(31)	1315(1)	11336(5)	1459(2)	68(1)
F(1)	346(1)	4542(4)	3357(2)	123(1)	C(32)	1609(1)	10993(6)	1223(3)	85(2)
F(2)	483(1)	4155(4)	4369(2)	146(2)	C(33)	1893(1)	11781(8)	1354(3)	104(2)
F(3)	560(1)	5994(5)	3961(2)	144(2)	C(34)	1885(2)	12868(8)	1733(4)	121(3)
F(4)	566(1)	8593(5)	-1667(2)	161(2)	C(35)	1599(2)	13203(7)	1969(3)	118(2)
F(5)	61(1)	8181(5)	-1787(2)	159(2)	C(36)	1315(1)	12434(6)	1829(3)	89(2)
F(6)	200(2)	10068(5)	-1746(2)	188(2)					
C(1)	1446(1)	3258(5)	4084(2)	61(1)					
C(2)	1446(1)	1811(5)	4020(2)	60(1)					
C(3)	1780(1)	104(5)	3607(3)	72(1)					
C(4)	1487(1)	-492(6)	3170(3)	97(2)					
C(5)	1868(1)	-592(5)	4257(3)	83(2)					
C(6)	2094(1)	214(6)	3262(3)	116(2)					
C(7)	923(1)	4362(6)	3718(3)	83(2)					
C(8)	579(1)	4752(7)	3868(3)	87(2)					
C(9)	1730(1)	3726(5)	4619(2)	65(1)					
C(10)	1645(1)	3382(6)	5300(2)	91(2)					
C(11)	1819(1)	5132(5)	4532(2)	69(1)					
C(12)	2074(2)	5659(6)	5105(3)	115(2)					
C(13)	1952(1)	5326(5)	3884(2)	62(1)					
C(14)	2243(1)	4699(5)	3751(3)	86(2)					
C(15)	2367(1)	4911(6)	3171(3)	100(2)					
C(16)	2205(1)	5737(6)	2707(3)	92(2)					
C(17)	1790(1)	6101(5)	3400(3)	72(1)					

Table 3. Bond lengths [Å] and angles [°] for **3f**.

O(1)-C(2)	1.332(4)	O(1)-C(3)-C(5)	109.5(4)	C(28)-C(27)-C(29)	112.3(4)
O(1)-C(3)	1.468(6)	C(4)-C(3)-C(5)	112.6(4)	C(28)-C(27)-C(19)	110.0(4)
O(2)-C(2)	1.195(5)	O(1)-C(3)-C(6)	101.9(4)	C(29)-C(27)-C(19)	113.9(3)
O(3)-C(7)	1.211(6)	C(4)-C(3)-C(6)	112.4(5)	N(4)-C(28)-C(27)	113.7(4)
O(4)-N(2)	1.182(6)	C(5)-C(3)-C(6)	110.1(4)	C(31)-C(29)-C(27)	110.3(3)
O(5)-N(2)	1.130(6)	O(3)-C(7)-N(1)	126.5(4)	C(31)-C(29)-C(30)	113.2(4)
N(1)-C(7)	1.314(6)	O(3)-C(7)-C(8)	117.9(5)	C(27)-C(29)-C(30)	113.0(3)
N(1)-C(1)	1.472(5)	N(1)-C(7)-C(8)	115.6(5)	C(36)-C(31)-C(32)	118.6(5)
N(2)-C(10)	1.429(7)	F(2)-C(8)-F(3)	109.0(6)	C(36)-C(31)-C(29)	123.1(4)
F(1)-C(8)	1.311(6)	F(2)-C(8)-F(1)	106.7(5)	C(32)-C(31)-C(29)	118.3(5)
F(2)-C(8)	1.303(6)	F(3)-C(8)-F(1)	103.3(5)	C(31)-C(32)-C(33)	119.7(6)
F(3)-C(8)	1.310(6)	F(2)-C(8)-C(7)	114.7(5)	C(34)-C(33)-C(32)	120.2(6)
C(1)-C(2)	1.510(6)	F(3)-C(8)-C(7)	111.5(5)	C(35)-C(34)-C(33)	120.4(6)
C(1)-C(9)	1.535(6)	F(1)-C(8)-C(7)	110.9(5)	C(34)-C(35)-C(36)	119.5(7)
C(3)-C(4)	1.500(7)	C(11)-C(9)-C(10)	115.0(4)	C(31)-C(36)-C(35)	121.7(6)
C(3)-C(5)	1.507(6)	C(11)-C(9)-C(1)	112.6(4)		
C(3)-C(6)	1.539(6)	C(10)-C(9)-C(1)	109.4(4)		
C(7)-C(8)	1.519(7)	N(2)-C(10)-C(9)	114.9(4)		
C(9)-C(11)	1.523(6)	C(13)-C(11)-C(9)	110.5(4)		
C(9)-C(10)	1.525(6)	C(13)-C(11)-C(12)	109.8(4)		
C(11)-C(13)	1.516(6)	C(9)-C(11)-C(12)	113.3(4)		
C(11)-C(12)	1.535(7)	C(17)-C(13)-C(14)	117.1(4)		
C(13)-C(17)	1.364(6)	C(17)-C(13)-C(11)	121.4(4)		
C(13)-C(14)	1.402(6)	C(14)-C(13)-C(11)	121.5(5)		
C(14)-C(15)	1.372(7)	C(15)-C(14)-C(13)	121.1(5)		
C(15)-C(16)	1.370(8)	C(16)-C(15)-C(14)	120.2(5)		
C(16)-C(18)	1.363(7)	C(18)-C(16)-C(15)	119.4(5)		
C(17)-C(18)	1.379(6)	C(13)-C(17)-C(18)	121.8(5)		
O(6)-C(20)	1.203(4)	C(16)-C(18)-C(17)	120.3(5)		
O(7)-C(20)	1.323(4)	C(20)-O(7)-C(21)	123.3(3)		
O(7)-C(21)	1.494(6)	O(9)-N(4)-O(10)	125.4(6)		
O(8)-C(25)	1.227(5)	O(9)-N(4)-C(28)	117.0(6)		
O(9)-N(4)	1.189(5)	O(10)-N(4)-C(28)	117.6(5)		
O(10)-N(4)	1.220(6)	C(25)-N(3)-C(19)	120.4(3)		
N(4)-C(28)	1.510(6)	N(3)-C(19)-C(20)	109.1(3)		
N(3)-C(25)	1.333(5)	N(3)-C(19)-C(27)	108.0(3)		
N(3)-C(19)	1.459(5)	C(20)-C(19)-C(27)	113.1(3)		
F(4)-C(26)	1.277(6)	O(6)-C(20)-O(7)	125.2(4)		
F(5)-C(26)	1.354(8)	O(6)-C(20)-C(19)	123.6(4)		
F(6)-C(26)	1.257(7)	O(7)-C(20)-C(19)	111.1(4)		
C(19)-C(20)	1.512(6)	C(24)-C(21)-O(7)	109.0(5)		
C(19)-C(27)	1.543(6)	C(24)-C(21)-C(23)	112.4(5)		
		O(7)-C(21)-C(23)	109.8(4)		
C(2)-O(1)-C(3)	122.3(3)	C(24)-C(21)-C(22)	110.5(5)		
C(7)-N(1)-C(1)	120.0(4)	O(7)-C(21)-C(22)	101.7(4)		
O(5)-N(2)-O(4)	120.7(7)	C(23)-C(21)-C(22)	112.8(5)		
O(5)-N(2)-C(10)	118.9(7)	O(8)-C(25)-N(3)	126.1(4)		
O(4)-N(2)-C(10)	120.4(6)	O(8)-C(25)-C(26)	120.1(5)		
N(1)-C(1)-C(2)	110.2(3)	N(3)-C(25)-C(26)	113.7(4)		
N(1)-C(1)-C(9)	113.1(4)	F(6)-C(26)-F(4)	113.2(6)		
C(2)-C(1)-C(9)	111.6(4)	F(6)-C(26)-F(5)	102.7(5)		
O(2)-C(2)-O(1)	126.0(5)	F(4)-C(26)-F(5)	102.6(6)		
O(2)-C(2)-C(1)	125.1(4)	F(6)-C(26)-C(25)	111.6(6)		
O(1)-C(2)-C(1)	108.9(4)	F(4)-C(26)-C(25)	115.5(5)		
O(1)-C(3)-C(4)	109.8(4)	F(5)-C(26)-C(25)	110.2(6)		

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **3f**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	62(2)	69(3)	103(2)	9(2)	47(2)	6(2)
O(2)	54(2)	74(3)	107(2)	14(2)	39(2)	-1(2)
O(3)	81(3)	227(6)	134(4)	107(4)	36(3)	40(3)
O(4)	240(7)	320(10)	128(5)	38(5)	11(5)	178(7)
O(5)	297(8)	403(12)	72(4)	28(5)	10(4)	160(8)
N(1)	42(2)	67(3)	70(2)	6(2)	9(2)	11(2)
N(2)	151(5)	177(7)	68(4)	22(4)	17(4)	57(4)
F(1)	62(2)	163(4)	138(3)	0(2)	-3(2)	11(2)
F(2)	75(2)	226(5)	148(3)	84(3)	55(2)	67(2)
F(3)	96(3)	120(4)	209(4)	-19(3)	-2(2)	32(2)
C(1)	43(2)	74(4)	70(3)	8(2)	23(2)	3(2)
C(2)	49(3)	64(4)	72(3)	7(3)	23(2)	4(2)
C(3)	62(3)	68(4)	92(4)	8(3)	37(3)	12(3)
C(4)	94(4)	100(5)	94(4)	-7(3)	5(3)	19(3)
C(5)	70(3)	69(4)	108(4)	11(3)	12(3)	10(3)
C(6)	106(4)	108(5)	156(6)	19(4)	89(4)	33(4)
C(7)	54(3)	100(5)	97(4)	29(3)	23(3)	11(3)
C(8)	58(3)	91(5)	109(5)	9(4)	7(3)	18(3)
C(9)	48(3)	81(4)	67(3)	11(3)	16(2)	2(2)
C(10)	51(3)	141(6)	78(4)	31(4)	2(3)	6(3)
C(11)	62(3)	65(4)	85(4)	0(3)	23(3)	4(2)
C(12)	128(5)	118(6)	91(4)	-21(4)	-6(4)	-28(4)
C(13)	51(3)	56(4)	81(3)	-1(3)	19(2)	-6(2)
C(14)	51(3)	92(5)	120(4)	13(3)	30(3)	2(3)
C(15)	60(3)	112(6)	141(5)	0(4)	53(4)	-2(3)
C(16)	79(4)	98(5)	108(5)	-7(4)	44(4)	-19(3)
C(17)	69(3)	64(4)	87(4)	-3(3)	28(3)	-2(3)
C(18)	90(4)	75(4)	87(4)	5(3)	28(3)	-8(3)
O(6)	59(2)	79(3)	70(2)	2(2)	28(2)	11(2)
O(7)	60(2)	77(3)	66(2)	8(2)	28(2)	4(2)
O(8)	48(2)	134(3)	85(2)	-28(2)	11(2)	13(2)
O(9)	157(4)	124(4)	181(4)	45(3)	120(4)	45(3)
O(10)	148(4)	82(4)	167(5)	6(3)	16(3)	-6(3)
N(4)	83(3)	76(4)	112(4)	19(3)	25(3)	19(3)
N(3)	46(2)	94(3)	50(2)	6(2)	8(2)	9(2)
F(4)	96(2)	328(6)	64(2)	-2(3)	27(2)	52(3)
F(5)	130(3)	253(6)	87(3)	-46(3)	-9(2)	31(3)
F(6)	310(6)	159(5)	91(3)	46(3)	18(3)	77(4)
C(19)	40(2)	67(4)	56(3)	3(2)	16(2)	12(2)
C(20)	38(2)	71(4)	55(3)	-5(2)	15(2)	-3(2)
C(21)	84(4)	77(5)	85(4)	23(3)	40(3)	3(3)
C(22)	158(6)	140(7)	117(5)	45(4)	91(5)	27(5)
C(23)	99(5)	153(7)	120(5)	65(5)	7(4)	21(4)
C(24)	150(6)	92(6)	157(6)	13(5)	60(5)	-32(5)
C(25)	63(3)	95(5)	59(3)	-8(3)	10(3)	29(3)
C(26)	81(4)	141(7)	65(4)	0(4)	-2(3)	25(4)
C(27)	45(2)	59(3)	66(3)	5(2)	22(2)	9(2)
C(28)	53(3)	66(4)	96(4)	15(3)	27(2)	8(2)
C(29)	49(2)	61(3)	67(3)	-1(2)	15(2)	1(2)
C(30)	62(3)	122(5)	73(3)	-19(3)	21(3)	2(3)
C(31)	62(3)	70(4)	71(3)	1(3)	3(2)	3(3)
C(32)	51(3)	100(5)	101(4)	6(3)	6(3)	-2(3)
C(33)	52(3)	139(7)	118(5)	21(5)	5(3)	-7(4)
C(34)	105(5)	138(8)	110(6)	9(5)	-15(4)	-49(5)
C(35)	127(6)	113(6)	110(5)	-18(4)	4(4)	-41(5)
C(36)	80(4)	91(5)	93(4)	-6(4)	4(3)	-11(3)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **3f**.

	x	y	z	U(eq)
H(1)	1491	3612	3661	73
H(4A)	1441	-15	2765	146
H(4B)	1293	-478	3392	146
H(4C)	1541	-1365	3074	146
H(5A)	2055	-174	4519	124
H(5B)	1926	-1466	4177	124
H(5C)	1677	-578	4490	124
H(6A)	2273	607	3558	174
H(6B)	2042	732	2872	174
H(6C)	2162	-628	3142	174
H(9)	1930	3226	4564	77
H(10A)	1578	4159	5507	109
H(10B)	1453	2804	5242	109
H(11)	1612	5636	4513	83
H(12A)	2117	6550	5028	172
H(12B)	2280	5183	5134	172
H(12C)	1984	5572	5512	172
H(14)	2354	4131	4061	103
H(15)	2561	4491	3093	121
H(16)	2293	5904	2320	110
H(17)	1590	6498	3465	86
H(18)	1798	6849	2496	99
H(19)	405	9691	442	64
H(22A)	474	7755	2340	196
H(22B)	396	6283	2377	196
H(22C)	167	7163	1874	196
H(23A)	1047	7415	2107	188
H(23B)	1113	6572	1505	188
H(23C)	1016	5915	2139	188
H(24A)	262	5692	1001	194
H(24B)	527	4841	1447	194
H(24C)	622	5502	812	194
H(27)	1082	10268	332	66
H(28A)	579	11653	-80	84
H(28B)	661	12215	637	84
H(29)	1087	9595	1418	70
H(30A)	545	10192	1595	127
H(30B)	651	11645	1617	127
H(30C)	815	10702	2172	127
H(32)	1617	10241	980	101
H(33)	2087	11569	1185	125
H(34)	2076	13377	1828	145
H(35)	1593	13942	2223	141
H(36)	1120	12670	1990	107

2-(Trifluoroacetyl)amino-3-cyano-4-phenylpentanoic acid *tert*-butylester (**4f**)

Table 1. Crystal data and structure refinement for **4f**.

Identification code	bm1
Empirical formula	C ₁₈ H ₂₁ F ₃ N ₂ O ₃
Formula weight	370.37
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P $\bar{1}$
Z	4
Unit cell dimensions	a = 10.8681(8) Å α = 80.628(1) deg. b = 10.9322(8) Å β = 89.495(1) deg. c = 16.0440(11) Å γ = 87.958(1) deg.
Volume	1879.6(2) Å ³
Density (calculated)	1.31 g/cm ³
Absorption coefficient	0.11 mm ⁻¹
Crystal shape	irregular
Crystal size	0.65 x 0.35 x 0.18 mm ³
Theta range for data collection	1.3 to 28.4 deg.
Index ranges	-14 ≤ h ≤ 14, -14 ≤ k ≤ 14, -21 ≤ l ≤ 21
Reflections collected	20025
Independent reflections	9283 (R(int) = 0.0323)
Observed reflections	7720 (I > 2σ(I))
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.98 and 0.93
Refinement method	Full-matrix least-squares on F ²
Data/restraints/parameters	9283 / 0 / 485
Goodness-of-fit on F ²	1.07
Final R indices (I > 2σ(I))	R1 = 0.037, wR2 = 0.100
Largest diff. peak and hole	0.38 and -0.38 eÅ ⁻³

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **4f**. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	$U(\text{eq})$
C12	0.1323(1)	0.8590(1)	0.1694(1)	0.0157(2)
C22	0.0893(1)	0.9877(1)	0.1875(1)	0.0162(2)
C32	-0.0014(1)	0.9790(1)	0.2632(1)	0.0174(2)
C42	-0.0772(1)	1.0996(1)	0.2625(1)	0.0254(2)
C52	0.0693(1)	0.9435(1)	0.3452(1)	0.0181(2)
C62	0.0593(1)	0.8279(1)	0.3951(1)	0.0226(2)
C72	0.1239(1)	0.7987(1)	0.4706(1)	0.0291(3)
C82	0.1986(1)	0.8846(1)	0.4969(1)	0.0325(3)
C92	0.2090(1)	0.9998(1)	0.4478(1)	0.0329(3)
C102	0.1449(1)	1.0290(1)	0.3727(1)	0.0254(2)
C112	0.2446(1)	0.8679(1)	0.1104(1)	0.0179(2)
O112	0.3025(1)	0.9603(1)	0.0935(1)	0.0259(2)
O122	0.2663(1)	0.7601(1)	0.0845(1)	0.0195(2)
C122	0.3649(1)	0.7435(1)	0.0217(1)	0.0229(2)
C132	0.3485(1)	0.6111(1)	0.0088(1)	0.0315(3)
C142	0.4900(1)	0.7592(1)	0.0589(1)	0.0292(3)
C152	0.3401(1)	0.8347(1)	-0.0590(1)	0.0322(3)
C162	0.0364(1)	1.0608(1)	0.1100(1)	0.0184(2)
N162	-0.0042(1)	1.1153(1)	0.0492(1)	0.0243(2)
C172	-0.0169(1)	0.6973(1)	0.1815(1)	0.0205(2)
O172	0.0089(1)	0.6503(1)	0.2534(1)	0.0273(2)
N172	0.0332(1)	0.7958(1)	0.1358(1)	0.0172(2)
H172	0.0147(13)	0.8152(13)	0.0839(10)	0.025(3)
C182	-0.1197(1)	0.6397(1)	0.1369(1)	0.0292(3)
F12	-0.0853(1)	0.5274(1)	0.1245(1)	0.0613(3)
F22	-0.1521(1)	0.7051(1)	0.0637(1)	0.0695(4)
F32	-0.2196(1)	0.6287(1)	0.1848(1)	0.0454(2)
C11	-0.5894(1)	0.5661(1)	0.3000(1)	0.0170(2)
C21	-0.6957(1)	0.5320(1)	0.3632(1)	0.0190(2)
C31	-0.7334(1)	0.3943(1)	0.3736(1)	0.0220(2)
C41	-0.8578(1)	0.3812(1)	0.4192(1)	0.0301(3)
C51	-0.7345(1)	0.3469(1)	0.2901(1)	0.0221(2)
C61	-0.6530(1)	0.2515(1)	0.2762(1)	0.0260(2)
C71	-0.6531(1)	0.2060(1)	0.2002(1)	0.0305(3)
C81	-0.7345(1)	0.2560(1)	0.1373(1)	0.0315(3)
C91	-0.8166(1)	0.3505(1)	0.1505(1)	0.0320(3)
C101	-0.8170(1)	0.3958(1)	0.2265(1)	0.0277(2)
C111	-0.5607(1)	0.7025(1)	0.2991(1)	0.0182(2)
O111	-0.6367(1)	0.7840(1)	0.2783(1)	0.0249(2)
O121	-0.4471(1)	0.7147(1)	0.3253(1)	0.0193(2)
C121	-0.4001(1)	0.8387(1)	0.3322(1)	0.0216(2)
C131	-0.3916(1)	0.9145(1)	0.2445(1)	0.0311(3)
C141	-0.4807(1)	0.9010(1)	0.3915(1)	0.0326(3)
C151	-0.2736(1)	0.8041(1)	0.3696(1)	0.0271(2)
C161	-0.6612(1)	0.5587(1)	0.4468(1)	0.0221(2)
N161	-0.6287(1)	0.5754(1)	0.5112(1)	0.0302(2)
C171	-0.4268(1)	0.4414(1)	0.2506(1)	0.0189(2)
O171	-0.4588(1)	0.4635(1)	0.1778(1)	0.0276(2)
N171	-0.4836(1)	0.4817(1)	0.3162(1)	0.0178(2)
H171	-0.4500(13)	0.4681(13)	0.3637(10)	0.028(4)
C181	-0.3143(1)	0.3539(1)	0.2752(1)	0.0231(2)
F11	-0.3499(1)	0.2432(1)	0.3140(1)	0.0486(2)
F21	-0.2502(1)	0.3363(1)	0.2081(1)	0.0358(2)
F31	-0.2387(1)	0.3962(1)	0.3274(1)	0.0384(2)

Table 3. Bond lengths [Å] and angles [°] for **4f**.

C12-N172	1.4535(13)				
C12-C112	1.5337(14)	N172-C12-C112	111.14(8)	O111-C111-O121	127.05(10)
C12-C22	1.5376(14)	N172-C12-C22	111.65(8)	O111-C111-C11	121.33(9)
C22-C162	1.4738(14)	C112-C12-C22	111.27(8)	O121-C111-C11	111.59(8)
C22-C32	1.5513(14)	C162-C22-C12	109.20(8)	C111-O121-C121	121.15(8)
C32-C52	1.5174(14)	C162-C22-C32	112.19(8)	O121-C121-C141	110.21(9)
C32-C42	1.5280(14)	C12-C22-C32	112.16(8)	O121-C121-C151	101.43(8)
C52-C62	1.3890(15)	C52-C32-C42	111.25(8)	C141-C121-C151	111.26(10)
C52-C102	1.3914(15)	C52-C32-C22	109.57(8)	O121-C121-C131	108.95(9)
C62-C72	1.3919(16)	C42-C32-C22	111.84(9)	C141-C121-C131	112.91(10)
C72-C82	1.3814(19)	C62-C52-C102	118.55(10)	C151-C121-C131	111.46(10)
C82-C92	1.380(2)	C62-C52-C32	121.72(10)	N161-C161-C21	176.22(11)
C92-C102	1.3834(16)	C102-C52-C32	119.72(10)	O171-C171-N171	126.35(10)
C112-O112	1.2014(13)	C52-C62-C72	120.42(11)	O171-C171-C181	119.42(10)
C112-O122	1.3245(13)	C82-C72-C62	120.27(11)	N171-C171-C181	114.16(9)
O122-C122	1.4913(12)	C92-C82-C72	119.69(11)	C171-N171-C11	118.75(9)
C122-C132	1.5119(17)	C82-C92-C102	120.13(12)	F21-C181-F31	107.51(10)
C122-C142	1.5156(16)	C92-C102-C52	120.94(11)	F21-C181-F11	107.68(10)
C122-C152	1.5197(16)	O112-C112-O122	127.46(10)	F31-C181-F11	106.87(10)
C162-N162	1.1403(14)	O112-C112-C12	122.81(9)	F21-C181-C171	111.03(9)
C172-O172	1.2145(14)	O122-C112-C12	109.72(8)	F31-C181-C171	112.95(9)
C172-N172	1.3312(14)	C112-O122-C122	121.70(8)	F11-C181-C171	110.55(9)
C172-C182	1.5389(15)	O122-C122-C132	102.00(9)		
C182-F22	1.3149(15)	O122-C122-C142	109.89(9)		
C182-F12	1.3169(16)	C132-C122-C142	111.40(10)		
C182-F32	1.3214(15)	O122-C122-C152	109.06(9)		
C11-N171	1.4465(13)	C132-C122-C152	111.58(10)		
C11-C111	1.5325(14)	C142-C122-C152	112.39(10)		
C11-C21	1.5449(14)	N162-C162-C22	178.60(11)		
C21-C161	1.4732(15)	O172-C172-N172	127.26(10)		
C21-C31	1.5568(15)	O172-C172-C182	117.82(10)		
C31-C51	1.5124(16)	N172-C172-C182	114.92(9)		
C31-C41	1.5309(16)	C172-N172-C12	121.07(9)		
C51-C61	1.3888(16)	F22-C182-F12	108.23(12)		
C51-C101	1.3912(16)	F22-C182-F32	107.15(11)		
C61-C71	1.3889(17)	F12-C182-F32	107.07(10)		
C71-C81	1.3803(19)	F22-C182-C172	113.71(10)		
C81-C91	1.3818(19)	F12-C182-C172	110.22(10)		
C91-C101	1.3880(17)	F32-C182-C172	110.21(10)		
C111-O111	1.2015(13)	N171-C11-C111	114.07(8)		
C111-O121	1.3255(12)	N171-C11-C21	112.63(8)		
O121-C121	1.4861(12)	C111-C11-C21	108.43(8)		
C121-C141	1.5134(16)	C161-C21-C11	109.38(9)		
C121-C151	1.5148(15)	C161-C21-C31	108.28(9)		
C121-C131	1.5172(17)	C11-C21-C31	114.78(8)		
C161-N161	1.1390(15)	C51-C31-C41	112.34(9)		
C171-O171	1.2056(13)	C51-C31-C21	112.13(9)		
C171-N171	1.3433(13)	C41-C31-C21	109.03(9)		
C171-C181	1.5391(15)	C61-C51-C101	118.58(11)		
C181-F21	1.3131(13)	C61-C51-C31	119.94(10)		
C181-F31	1.3253(14)	C101-C51-C31	121.47(10)		
C181-F11	1.3365(14)	C51-C61-C71	120.91(12)		
		C81-C71-C61	119.98(12)		
		C71-C81-C91	119.69(11)		
		C81-C91-C101	120.41(12)		
		C91-C101-C51	120.43(11)		

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **3f**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C12	0.0153(4)	0.0175(5)	0.0143(4)	-0.0027(4)	-0.0011(3)	0.0008(3)
C22	0.0166(4)	0.0178(5)	0.0139(4)	-0.0018(4)	-0.0013(3)	0.0011(4)
C32	0.0161(5)	0.0212(5)	0.0148(5)	-0.0029(4)	-0.0001(4)	0.0011(4)
C42	0.0257(6)	0.0276(6)	0.0220(5)	-0.0035(4)	0.0018(4)	0.0087(4)
C52	0.0167(5)	0.0235(5)	0.0141(5)	-0.0037(4)	0.0019(4)	0.0029(4)
C62	0.0198(5)	0.0257(5)	0.0213(5)	-0.0016(4)	0.0020(4)	0.0023(4)
C72	0.0264(6)	0.0363(6)	0.0205(5)	0.0054(5)	0.0035(4)	0.0078(5)
C82	0.0264(6)	0.0549(8)	0.0150(5)	-0.0039(5)	-0.0031(4)	0.0063(5)
C92	0.0317(6)	0.0476(8)	0.0221(6)	-0.0130(5)	-0.0041(5)	-0.0054(5)
C102	0.0293(6)	0.0277(6)	0.0199(5)	-0.0053(4)	-0.0008(4)	-0.0032(4)
C112	0.0173(5)	0.0212(5)	0.0150(5)	-0.0026(4)	-0.0013(4)	0.0022(4)
O112	0.0244(4)	0.0237(4)	0.0298(4)	-0.0049(3)	0.0081(3)	-0.0037(3)
O122	0.0197(4)	0.0226(4)	0.0169(4)	-0.0055(3)	0.0031(3)	0.0016(3)
C122	0.0212(5)	0.0318(6)	0.0152(5)	-0.0045(4)	0.0040(4)	0.0059(4)
C132	0.0364(7)	0.0344(6)	0.0257(6)	-0.0127(5)	0.0030(5)	0.0069(5)
C142	0.0212(5)	0.0408(7)	0.0248(6)	-0.0041(5)	0.0028(4)	0.0044(5)
C152	0.0339(6)	0.0428(7)	0.0173(5)	0.0002(5)	0.0027(5)	0.0102(5)
C162	0.0198(5)	0.0184(5)	0.0173(5)	-0.0044(4)	0.0000(4)	0.0005(4)
N162	0.0289(5)	0.0235(5)	0.0200(5)	-0.0023(4)	-0.0033(4)	0.0022(4)
C172	0.0222(5)	0.0192(5)	0.0206(5)	-0.0047(4)	0.0006(4)	-0.0009(4)
O172	0.0380(5)	0.0228(4)	0.0200(4)	0.0007(3)	-0.0010(3)	-0.0054(3)
N172	0.0176(4)	0.0193(4)	0.0145(4)	-0.0019(3)	-0.0026(3)	-0.0005(3)
C182	0.0303(6)	0.0304(6)	0.0275(6)	-0.0043(5)	-0.0009(5)	-0.0102(5)
F12	0.0461(5)	0.0516(6)	0.0994(8)	-0.0502(6)	-0.0066(5)	-0.0069(4)
F22	0.0745(7)	0.0861(8)	0.0419(5)	0.0206(5)	-0.0327(5)	-0.0552(6)
F32	0.0283(4)	0.0587(5)	0.0529(5)	-0.0172(4)	0.0067(4)	-0.0153(4)
C11	0.0170(5)	0.0200(5)	0.0140(4)	-0.0034(4)	-0.0022(4)	0.0019(4)
C21	0.0189(5)	0.0222(5)	0.0158(5)	-0.0036(4)	-0.0006(4)	0.0017(4)
C31	0.0230(5)	0.0221(5)	0.0200(5)	-0.0004(4)	0.0005(4)	-0.0003(4)
C41	0.0284(6)	0.0330(6)	0.0280(6)	-0.0017(5)	0.0066(5)	-0.0046(5)
C51	0.0227(5)	0.0203(5)	0.0235(5)	-0.0031(4)	0.0024(4)	-0.0051(4)
C61	0.0222(5)	0.0234(5)	0.0326(6)	-0.0050(5)	0.0013(4)	-0.0039(4)
C71	0.0267(6)	0.0264(6)	0.0414(7)	-0.0138(5)	0.0078(5)	-0.0060(5)
C81	0.0353(7)	0.0322(6)	0.0306(6)	-0.0136(5)	0.0067(5)	-0.0135(5)
C91	0.0375(7)	0.0314(6)	0.0280(6)	-0.0061(5)	-0.0052(5)	-0.0063(5)
C101	0.0302(6)	0.0249(6)	0.0285(6)	-0.0060(5)	-0.0033(5)	0.0002(5)
C111	0.0181(5)	0.0220(5)	0.0148(5)	-0.0041(4)	-0.0022(4)	0.0006(4)
O111	0.0213(4)	0.0228(4)	0.0306(4)	-0.0050(3)	-0.0077(3)	0.0035(3)
O121	0.0166(3)	0.0196(4)	0.0220(4)	-0.0040(3)	-0.0038(3)	-0.0004(3)
C121	0.0208(5)	0.0203(5)	0.0246(5)	-0.0059(4)	-0.0026(4)	-0.0031(4)
C131	0.0346(6)	0.0265(6)	0.0305(6)	0.0018(5)	-0.0051(5)	-0.0060(5)
C141	0.0277(6)	0.0346(6)	0.0403(7)	-0.0204(6)	0.0005(5)	-0.0014(5)
C151	0.0204(5)	0.0318(6)	0.0298(6)	-0.0059(5)	-0.0042(4)	-0.0040(4)
C161	0.0214(5)	0.0259(5)	0.0187(5)	-0.0037(4)	0.0012(4)	0.0061(4)
N161	0.0300(5)	0.0416(6)	0.0196(5)	-0.0085(4)	-0.0026(4)	0.0111(4)
C171	0.0202(5)	0.0182(5)	0.0178(5)	-0.0022(4)	0.0001(4)	0.0010(4)
O171	0.0314(4)	0.0352(5)	0.0151(4)	-0.0035(3)	-0.0006(3)	0.0095(3)
N171	0.0192(4)	0.0203(4)	0.0139(4)	-0.0034(3)	-0.0034(3)	0.0033(3)
C181	0.0243(5)	0.0232(5)	0.0205(5)	-0.0011(4)	0.0004(4)	0.0037(4)
F11	0.0329(4)	0.0309(4)	0.0713(6)	0.0217(4)	0.0022(4)	0.0064(3)
F21	0.0391(4)	0.0413(4)	0.0266(4)	-0.0091(3)	0.0040(3)	0.0190(3)
F31	0.0261(4)	0.0555(5)	0.0370(4)	-0.0203(4)	-0.0115(3)	0.0143(3)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for **4f**.

	x	y	z	U(eq)
H12	0.1582	0.8081	0.2243	0.019
H22	0.1636	1.0308	0.2025	0.019
H32	-0.0595	0.9116	0.2586	0.021
H4A2	-0.1267	1.0939	0.3142	0.038
H4B2	-0.1318	1.1133	0.2132	0.038
H4C2	-0.0218	1.1690	0.2594	0.038
H62	0.0080	0.7684	0.3775	0.027
H72	0.1165	0.7193	0.5043	0.035
H82	0.2427	0.8645	0.5484	0.039
H92	0.2604	1.0591	0.4656	0.039
H102	0.1524	1.1086	0.3394	0.030
H13A2	0.3621	0.5551	0.0624	0.047
H13B2	0.4079	0.5899	-0.0333	0.047
H13C2	0.2647	0.6024	-0.0111	0.047
H14A2	0.4976	0.8455	0.0670	0.044
H14B2	0.5547	0.7377	0.0203	0.044
H14C2	0.4985	0.7044	0.1135	0.044
H15A2	0.2542	0.8300	-0.0759	0.048
H15B2	0.3947	0.8139	-0.1040	0.048
H15C2	0.3555	0.9190	-0.0492	0.048
H172	0.0147(13)	0.8152(13)	0.0839(10)	0.025(3)
H11	-0.6206	0.5591	0.2426	0.020
H21	-0.7694	0.5858	0.3432	0.023
H31	-0.6708	0.3430	0.4105	0.026
H4A1	-0.9212	0.4299	0.3840	0.045
H4B1	-0.8524	0.4117	0.4732	0.045
H4C1	-0.8793	0.2937	0.4296	0.045
H61	-0.5965	0.2170	0.3192	0.031
H71	-0.5971	0.1404	0.1917	0.037
H81	-0.7341	0.2257	0.0850	0.038
H91	-0.8731	0.3846	0.1074	0.038
H101	-0.8740	0.4605	0.2350	0.033
H13A1	-0.3404	0.8690	0.2084	0.047
H13B1	-0.3546	0.9940	0.2480	0.047
H13C1	-0.4743	0.9297	0.2203	0.047
H14A1	-0.5601	0.9265	0.3644	0.049
H14B1	-0.4401	0.9742	0.4046	0.049
H14C1	-0.4941	0.8428	0.4438	0.049
H15A1	-0.2822	0.7533	0.4255	0.041
H15B1	-0.2306	0.8797	0.3750	0.041
H15C1	-0.2263	0.7569	0.3325	0.041
H171	-0.4500(13)	0.4681(13)	0.3637(10)	0.028(4)