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Supporting Information:

(±)-**Trans-2-Fluorocyclohexyl-N-phenylcarbamate 3**. ^1H NMR: δ 1.21-1.85 (m, 6H, $-\text{CH}_2$), 2.04-2.23 (m, 2H, $-\text{CH}_2$), 4.44 (dddd, $^2J_{\text{H,F}} = 50.3$ Hz, $^3J_{\text{Ha,Ha}} = 10.3$ Hz, $^3J_{\text{Ha,Ha}} = 8.4$ Hz, $^3J_{\text{Ha,He}} = 4.8$ Hz, 1H, 2-CH), 4.79-4.90 (m, 1H, 1-CH), 6.77 (br s, 1H, NH), 7.05 (t, $^3J_{\text{H,H}} = 7.3$ Hz, 1H, 11-CH), 7.27 (t, $^3J_{\text{H,H}} = 7.9$ Hz, 2H, 10-CH, 12-CH), 7.38 (br d, $^3J_{\text{H,H}} = 7.6$ Hz, 2H, 9-CH, 13-CH). ^{13}C NMR: δ 22.8 (dt, $^3J_{\text{C,F}} = 10.2$ Hz, C-4), 23.0 (t, C-5), 29.7 (dt, $^3J_{\text{C,F}} = 7.6$ Hz, C-6), 30.4 (dt, $^2J_{\text{C,F}} = 17.8$ Hz, C-3), 75.1 (dd, $^2J_{\text{C,F}} = 20.4$ Hz, C-1), 92.1 (dd, $^1J_{\text{C,F}} = 178.0$ Hz, C-2), 118.7 (2d, C-9, C-13), 123.4 (d, C-11), 129.0 (2d, C-10, C-12), 137.8 (s, C-8), 152.8 (s, C-7). ^{19}F NMR: δ -181.7 (d, $^2J_{\text{F,H}} = 47.7$ Hz, 2-CHF). GC-MS m/z : 237 (46) [M^+], 150 (5), 138 (4), 137 (23) [$\text{C}_6\text{H}_5\text{NHCO}_2\text{H}^+$], 132 (18), 119 (58) [$137 - \text{H}_2\text{O}$], 118 (7) [$\text{C}_6\text{H}_{11}\text{O}^+$], 94 (8), 93 (100) [$\text{C}_6\text{H}_5\text{NH}_2^+$], 91 (22), 81 (56) [C_6H_9^+], 77 (17) [C_6H_5^+], 72 (9), 64 (14), 59 (20), 57 (53) [C_4H_9^+], 55 (21), 51 (10), 41 (35) [C_3H_5^+].

(±)-**Trans-2-Fluorocycloheptyl-N-phenylcarbamate 6**. ^1H NMR: δ 1.38-2.05 (m, 10H, $-\text{CH}_2$), 4.62 (dm, $^2J_{\text{H,F}} = 48.4$ Hz, 1H, 2-CH), 4.90-5.06 (m, 1H, 1-CH), 6.56 (br s, 1H, NH), 7.04 (tt, $^3J_{\text{H,H}} = 6.9$ Hz, $^4J_{\text{H,H}} = 1.3$ Hz, 1H, 12-CH), 7.28 (t, $^3J_{\text{H,H}} = 8.0$ Hz, 2H, 11-CH, 13-CH), 7.36 (dd, $^3J_{\text{H,H}} = 8.6$ Hz, $^4J_{\text{H,H}} = 1.0$ Hz, 2H, 10-CH, 14-CH). ^{13}C NMR: δ 21.8 (dt, $^3J_{\text{C,F}} = 7.6$ Hz, C-4), 23.1 (t, C-6), 28.3 (t, C-5), 29.8 (dt, $^3J_{\text{C,F}} = 7.6$ Hz, C-7), 30.9 (dt, $^2J_{\text{C,F}} = 20.3$ Hz, C-3), 78.7 (dd, $^2J_{\text{C,F}} = 22.9$ Hz, C-1), 95.8 (dd, $^1J_{\text{C,F}} = 172.9$ Hz, C-2), 118.8 (2d, C-10, C-14), 123.5 (d, C-12), 129.1 (2d, C-11, C-13), 137.9 (s, C-9), 152.9 (s, C-8). ^{19}F NMR: δ -171.7 (m, 2-CHF). GC-MS, m/z :

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252 (6) [$M^+ + 1$], 251 (37) [M^+], 231 (4) [$M^+ - HF$], 138 (6), 137 (45) [$C_6H_5NHCO_2H^+$], 124 (13), 119 (26) [$137 - H_2O$], 95 (53), 93 (100) [$C_6H_5NH_2^+$], 91 (11), 77 (15) [$C_6H_5^+$], 73 (19), 67 (13), 57 (18), 55 (28) [$C_4H_7^+$], 43 (7), 41 (23) [$C_3H_5^+$].

(1R,2R,4R)-(-)-2-Fluoro-4-hydroxycyclohexyl-N-phenylcarbamate (-)-9. 1H NMR: δ 1.31-2.48 (m, 6H, $-CH_2$), 3.67- 3.83 (m, 1H, 4-CH), 4.49 (dddd, $^2J_{H,F} = 49.8$ Hz, $^3J_{Ha,Ha} = 10.7$ Hz, $^3J_{Ha,Ha} = 8.4$ Hz, $^3J_{Ha,He} = 4.8$ Hz, 1H, 2-CH), 4.79-4.93 (m, 1H, 1-CH), 6.57 (br. s, 1H, NH), 7.05 (tt, $^3J_{H,H} = 7.2$ Hz, $^4J_{H,H} = 1.4$ Hz, 1H, 11-CH), 7.29 (t, $^3J_{H,H} = 8.0$ Hz, 2H, 10-CH, 12-CH), 7.36 (dd, $^3J_{H,H} = 7.9$ Hz, $^4J_{H,H} = 1.2$ Hz, 2H, 9-CH, 13-CH). ^{13}C NMR: δ 25.0 (dt, $^3J_{C,F} = 5.1$ Hz, C-6), 32.0 (t, C-5), 39.0 (dt, $^2J_{C,F} = 15.3$ Hz, C-3), 67.3 (dt, $^3J_{C,F} = 10.1$ Hz, C-4), 74.4 (dd, $^2J_{C,F} = 20.3$ Hz, C-1), 89.9 (dd, $^1J_{C,F} = 180.6$ Hz, C-2), 118.8 (2d, C-9, C-13), 123.7 (d, C-11), 129.1 (2d, C-10, C-12), 137.6 (s, C-8), 152.7 (s, C-7). ^{19}F NMR: $\delta -183.2$ (m, 2-CHF). GC-MS, m/z : 254 (4) [$M^+ + 1$], 253 (29) [M^+], 138 (4), 137 (16) [$C_6H_5NHCO_2H^+$], 120 (6), 119 (22), 99 (56) [$C_6H_8F^+$], 93 (100) [$C_6H_5NH_2^+$], 79 (17) [$C_6H_7^+$], 77 (17) [$C_6H_5^+$], 73 (18), 65 (15), 55 (10), 43 (9), 41 (30) [$C_3H_5^+$].

(1S,2S,4R)-(+)-2-Fluoro-4-hydroxycyclohexyl-N-phenylcarbamate (+)-10. 1H NMR: δ 1.50-2.21 (m, 6H, 3- CH_2 , 5- CH_2 , 6- CH_2), 4.09-4.20 (m, 1H, 4-CH), 4.82 (dddd, $^2J_{H,F} = 33.6$ Hz, $^3J_{Ha,Ha} = 8.6$ Hz, $^3J_{Ha,Ha} = 7.4$ Hz, $^3J_{Ha,He} = 4.3$ Hz, 1H, 2-CH), 4.81-4.98 (m, 1H, 1-CH), 6.69 (br s, 1H, NH), 7.05 (tt, $^3J_{H,H} = 7.3$ Hz, $^4J_{H,H} = 1.4$ Hz, 1H, 11-CH), 7.29 (tt, $^3J_{H,H} = 7.9$ Hz, $^4J_{H,H} = 1.9$ Hz, 2H, 10-CH, 12-CH), 7.37 (dd,

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$^3J_{\text{H,H}} = 8.5$ Hz, $^4J_{\text{H,H}} = 1.2$ Hz, 2H, 9-CH, 13-CH). ^{13}C NMR: δ 24.2 (dt, $^3J_{\text{C,F}} = 3.9$ Hz, C-6), 30.0 (t, C-5), 36.9 (dt, $^2J_{\text{C,F}} = 18.5$ Hz, C-3), 66.1 (dt, $^3J_{\text{C,F}} = 8.7$ Hz, C-4), 73.1 (dd, $^2J_{\text{C,F}} = 21.6$ Hz, C-1), 89.5 (dd, $^1J_{\text{C,F}} = 174.9$ Hz, C-2), 118.7 (2d, C-9, C-13), 123.6 (d, C-11), 129.1 (2d, C-10, C-12), 137.7 (s, C-8), 152.7 (s, C-7). ^{19}F NMR: δ -189.0 (m, 2-CHF). GC-MS, m/z : 254 (6) [$\text{M}^+ + 1$], 253 (38) [M^+], 138 (4), 137 (20) [$\text{C}_6\text{H}_5\text{NHCO}_2\text{H}^+$], 120 (7), 119 (46), 117 (2), 99 (26) [$\text{C}_6\text{H}_{11}\text{O}^+$], 93 (100) [$\text{C}_6\text{H}_5\text{NH}_2^+$], 91 (5), 77 (16) [C_6H_5^+], 69 (14), 65 (8), 57 (7), 43 (6), 41 (24) [C_3H_5^+].

(1R,2R)-(-)-2-Fluorocyclohexyl-N-(p-hydroxyphenyl)carbamate (-)-13. ^1H NMR: δ 1.18-1.82 (m, 6H, $-\text{CH}_2$), 2.02-2.20 (m, 2H, $-\text{CH}_2$), 4.42 (dddd, $^2J_{\text{H,F}} = 50.5$ Hz, $^3J_{\text{Ha,Ha}} = 10.2$ Hz, $^3J_{\text{Ha,Ha}} = 8.4$ Hz, $^3J_{\text{Ha,He}} = 4.8$ Hz, 1H, 2-CH), 4.72-4.88 (m, 1H, 1-CH), 6.50 (br s, 1H, NH), 6.73 (dt, $^3J_{\text{H,H}} = 9.5$ Hz, $^4J_{\text{H,H}} = 2.8$ Hz, 2H, 10-CH, 12-CH), 7.17 (br d, $^3J_{\text{H,H}} = 8.8$ Hz, 2H, 9-CH, 13-CH). ^{13}C NMR: δ 22.9 (dt, $^3J_{\text{C,F}} = 7.5$ Hz, C-4), 23.1 (t, C-5), 29.8 (dt, $^3J_{\text{C,F}} = 5.1$ Hz, C-6), 30.5 (dt, $^2J_{\text{C,F}} = 17.8$ Hz, C-3), 75.2 (dd, $^2J_{\text{C,F}} = 17.8$ Hz, C-1), 92.2 (dd, $^1J_{\text{C,F}} = 178.0$ Hz, C-2), 115.8 (2d, C-10, C-12), 121.6 (2d, C-9, C-13), 130.5 (s, C-8), 152.5 (s, C-11) 153.7 (s, C-7). ^{19}F NMR: δ -181.7 (d, $^2J_{\text{F,H}} = 50.5$ Hz, 2-CHF). GC-MS, m/z : 255 (0.5), 254 (10) [$\text{M}^+ + 1$], 253 (77) [M^+], 154 (4), 153 (63) [$\text{C}_6\text{H}_4\text{OHNHCO}_2\text{H}^+$], 140 (12), 135 (22), 110 (8), 109 (100) [$\text{C}_6\text{H}_4\text{OHNH}_2^+$], 108 (24), 107 (6), 82 (7), 81 (71) [C_6H_9^+], 79 (10), 65 (4), 59 (16), 55 (21), 53 (15), 52 (9), 51 (4), 41 (38) [C_3H_5].

(-)-*Trans*-2-Fluorocyclohexyl-*N*-[*p*-(4'-methyl- β -D-glucopyranosyl)]phenyl-

carbamate (-)-14. ^1H NMR: δ 1.26-2.25 (m, 8H, -CH₂), 3.23 (dd, $^3J_{\text{Ha,Ha}} = 9.8$ Hz, $^3J_{\text{Ha,Ha}} = 9.5$ Hz, 1H, 16-CH), 3.38-3.94 (m, 6H, -CH, -CH₂), 3.63 (s, 3H, -CH₃), 4.50 (dddd, $^2J_{\text{H,F}} = 50.3$ Hz, $^3J_{\text{Ha,Ha}} = 10.0$ Hz, $^3J_{\text{Ha,Ha}} = 8.6$ Hz, $^3J_{\text{Ha,He}} = 4.8$ Hz, 1H, 2-CH), 4.69-4.89 (m, 1H, 1-CH), 7.08 (dt, $^3J_{\text{H,H}} = 9.1$ Hz, $^4J_{\text{H,H}} = 2.7$ Hz, 2H, 10-CH, 12-CH), 7.37 (br d, $^3J_{\text{H,H}} = 8.8$ Hz, 2H, 9-CH, 13-CH). ^{13}C NMR: δ 24.1 (dt, $^3J_{\text{C,F}} = 10.2$ Hz, C-4), 24.4 (t, C-5), 31.0 (dt, $^3J_{\text{C,F}} = 5.1$ Hz, C-6), 31.8 (dt, $^2J_{\text{C,F}} = 17.8$ Hz, C-3), 61.1 (q, C-20), 62.4 (t, C-19), 75.3, 77.4, 78.3, 80.9 (4d, C-15, C-16, C-17, C-18), 72.2 (dd, $^2J_{\text{C,F}} = 20.3$ Hz, C-1), 93.6 (dd, $^1J_{\text{C,F}} = 175.5$ Hz, C-2), 103.0 (d, C-14), 118.6 (2d, C-10, C-12), 121.8 (2d, C-9, C-13), 135.0 (s, C-8), 155.3 (s, C-11) 155.9 (s, C-7). ^{19}F NMR: δ -180.9 (d, $^2J_{\text{F,H}} = 53.4$ Hz, 2-CHF). ESI-MS, nanospray, m/z : 474 (40) [(M⁺ - H) + COOH]⁻, 428 (100) [M - H]⁻, 310 (18) [(M - H) - C₆H₁₁OF]⁻, 133 (13) [310 - C₇H₁₃O₅].

(-)-*Trans*-2-Fluorocyclohexyl-*N*-[*p*-(4'-methyl- β -D-glucopyranoacetyl)]-

phenylcarbamate. ^1H NMR: δ 1.15-2.18 (m, 8H, -CH₂), 2.03 (s, 3H, -CH₃), 2.06 (s, 3H, -CH₃), 2.07 (s, 3H, -CH₃), 3.42 (t, $^3J_{\text{Ha,Ha}} = 7.1$ Hz, 1H, 16-CH), 3.42 (s, 3H, 20-CH₃), 3.56-3.69 (m, 1H, 15-CH), 4.24 (dd, $J_{\text{H,H}} = 11.9$ Hz, $J_{\text{H,H}} = 5.5$ Hz, 1H, 19-CH₂), 4.39 (dd, $J_{\text{H,H}} = 11.9$ Hz, $J_{\text{H,H}} = 2.4$ Hz, 1H, 19-CH₂), 4.41 (dddd, $^2J_{\text{H,F}} = 52.6$ Hz, $^3J_{\text{Ha,Ha}} = 10.3$ Hz, $^3J_{\text{Ha,Ha}} = 8.3$ Hz, $^3J_{\text{Ha,He}} = 4.8$ Hz, 1H, 2-CH), 4.72-4.86 (m, 1H, 1-CH), 4.94 (d, $^3J_{\text{Ha,Ha}} = 7.6$ Hz, 1H, 14-CH), 5.10 (dd, $^3J_{\text{Ha,Ha}} = 9.5$ Hz, $^3J_{\text{Ha,Ha}} = 7.6$ Hz, 1H, 18-CH), 5.21 (t, $^3J_{\text{Ha,Ha}} = 9.2$ Hz, 1H, 17-CH), 6.59 (br s, 1H, NH), 6.91 (dt,

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$^3J_{\text{H,H}} = 9.1$ Hz, $^4J_{\text{H,H}} = 2.7$ Hz, 2H, 10-CH, 12-CH), 7.26 (br d, $^3J_{\text{H,H}} = 9.1$ Hz, 2H, 9-H, 13-CH). ^{13}C NMR: δ 20.7, 20.8, 20.9 (3q, -OCOCH₃), 22.9 (dt, $^3J_{\text{C,F}} = 10.1$ Hz, C-4), 23.1 (t, C-5), 29.8 (dt, $^3J_{\text{C,F}} = 5.8$ Hz, C-6), 30.5 (dt, $^2J_{\text{C,F}} = 18.4$ Hz, C-3), 60.3 (q, C-20), 62.8 (t, C-19), 71.8 (d, C-18), 73.1 (d, C-15), 74.9 (d, C-17), 77.7 (d, 16-CH), 75.3 (d, C-1), 92.2 (dd, $^1J_{\text{C,F}} = 178.1$ Hz, C-2), 99.6 (d, C-14), 117.9 (2d, C-10, C-12), 118.9 (2d, C-9, C-13), 132.3 (s, C-8), 153.0 (s, C-11) 153.2 (s, C-7), 169.7, 170.0, 170.6, (3s, -OCOCH₃). ^{19}F NMR: δ -181.8 (d, $^2J_{\text{F,H}} = 53.4$ Hz, 2-CHF). ESI-MS, nanospray, m/z : 554 (12) [M - H]⁻, 437 (25) [(M - H) - C₆H₁₀OF]⁻, 436 (100) [(M - H) - C₆H₁₁OF]⁻, 394 (8) [436 - C₂H₂O], 352 (5) [394 - C₂H₂O], 301 (13) [(M - H) - C₆H₁₁OFOCOHC₆H₅]⁻, 232 (13).

***Cis-* and *trans*-2-Fluoro-4-hydroxycyclohexyl-*N*-(*p*-hydroxyphenyl)carbamates **11** and **12**.** In the proton decoupled ^{19}F NMR spectra of the crude product mixtures of biotransformations of **3** two more signals, $\delta = -182.7$ and $\delta = -188.7$ ppm, were detected (both <1% of the total integral of all fluorinated compounds) which are located very close to the signals of products **9** (-183.2) and **10** (-189.0), respectively. These signals we assign to compounds **11** and **12**, respectively. The structures of these compounds are supported by the fact that in the mass spectra of a silylated sample of the crude product mixture (after treatment with *N*-methyl-*N*-trimethylsilyl-trifluoroacetamide) the molecular ions of the disilylated compounds **11** and **12** were identified. Compound **11**: GC-MS, m/z : 415 (8) [M⁺], 414 (10) [M⁺ - 1], 413 (27), 282 (5), 225 (20), 207 (100) [OCNC₆H₄OSiMe₃⁺], 192 (21) [207 - CH₃], 181 (13), 180 (6), 134 (4), 111 (4), 99 (10) [C₆H₈F⁺], 97 (6), 79 (11) [C₆H₇⁺], 75 (16), 73 (43) [SiMe₃⁺],

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69 (7), 45 (9). Compound **12**: GC-MS, m/z : 413 (27), 304 (2), 303 (8), 253 (21), 225 (18), 207 (34) [OCNC₆H₄OSiMe₃⁺], 192 (75) [207 - CH₃], 189 (27) [C₆H₉FOSiMe₃⁺], 169 (39), 129 (8), 107 (10), 99 (57) [C₆H₈F⁺], 97 (72), 79 (83) [C₆H₇⁺], 73 (100) [SiMe₃⁺], 69 (36), 67 (16), 55 (14), 41 (19) [C₃H₃⁺].

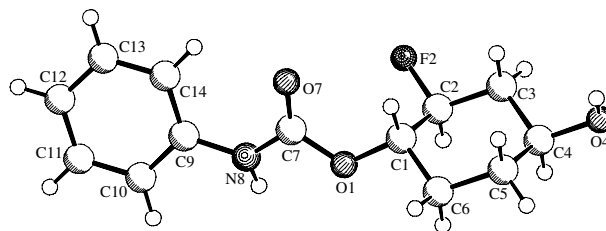


Figure 1. X-ray structure of (1*S*,2*S*,4*S*)-(+)-2-fluoro-4-hydroxycyclohexyl-*N*-phenylcarbamate ((*S,S,S*)-(+)-**9**)

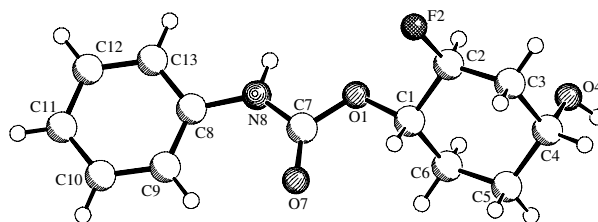


Figure 2 X-ray structure of (1*S*,2*S*,4*R*)-(+)-2-fluoro-4-hydroxycyclohexyl-*N*-phenylcarbamate ((*S,S,S*)-(+)-**10**)

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C1 C 0.3482(3) -0.0669(2) 0.06511(17) 0.0341(5) Uani 1 1 d . . .
H1 H 0.2862 -0.1327 0.0864 0.041 Uiso 1 1 calc R . .
C2 C 0.5003(3) -0.1131(2) 0.05537(17) 0.0368(5) Uani 1 1 d . . .
H2 H 0.5635 -0.0445 0.0418 0.044 Uiso 1 1 calc R . .
F2 F 0.56208(19) -0.16837(18) 0.15213(12) 0.0585(5) Uani 1 1 d . . .
C3 C 0.4962(3) -0.2026(2) -0.03554(18) 0.0369(5) Uani 1 1 d . . .
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S11

H3A H 0.4398 -0.2737 -0.0204 0.044 Uiso 1 1 calc R . .
H3B H 0.5971 -0.2283 -0.0409 0.044 Uiso 1 1 calc R . .
C4 C 0.4249(2) -0.14684(19) -0.14180(17) 0.0312(4) Uani 1 1 d
H4 H 0.4859 -0.0773 -0.1567 0.037 Uiso 1 1 calc R . .
O4 O 0.42191(19) -0.23084(14) -0.22836(12) 0.0382(4) Uani 1 1 d
H4A H 0.3578 -0.2825 -0.2243 0.057 Uiso 1 1 calc R . .
C5 C 0.2710(2) -0.1011(2) -0.13326(17) 0.0356(5) Uani 1 1 d
H5A H 0.2075 -0.1691 -0.1216 0.043 Uiso 1 1 calc R . .
H5B H 0.2284 -0.0621 -0.2009 0.043 Uiso 1 1 calc R . .
C6 C 0.2755(3) -0.0117(2) -0.04062(18) 0.0384(5) Uani 1 1 d
H6A H 0.3307 0.0599 -0.0558 0.046 Uiso 1 1 calc R . .
H6B H 0.1745 0.0131 -0.0345 0.046 Uiso 1 1 calc R . .
O1 O 0.3637(2) 0.02773(15) 0.14525(13) 0.0411(4) Uani 1 1 d
C7 C 0.3476(3) -0.0018(2) 0.24688(18) 0.0363(5) Uani 1 1 d
O7 O 0.3024(2) -0.09818(18) 0.27247(15) 0.0546(5) Uani 1 1 d
N8 N 0.3896(2) 0.09155(19) 0.31232(15) 0.0378(4) Uani 1 1 d
H8 H 0.429(3) 0.145(3) 0.284(2) 0.045 Uiso 1 1 d
C9 C 0.3854(2) 0.0972(2) 0.42387(17) 0.0344(4) Uani 1 1 d
C10 C 0.3988(3) 0.2093(2) 0.47223(19) 0.0398(5) Uani 1 1 d
H10 H 0.4084 0.2781 0.4307 0.048 Uiso 1 1 calc R . .
C11 C 0.3980(3) 0.2200(3) 0.5824(2) 0.0455(6) Uani 1 1 d
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C12 C 0.3834(3) 0.1199(3) 0.64440(19) 0.0500(7) Uani 1 1 d
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C13 C 0.3710(3) 0.0085(3) 0.5958(2) 0.0488(6) Uani 1 1 d
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C14 C 0.3721(3) -0.0040(2) 0.48622(19) 0.0414(5) Uani 1 1 d
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C21 C 0.1436(2) 0.5789(2) 0.59228(16) 0.0357(5) Uani 1 1 d
H21 H 0.2199 0.6346 0.6285 0.043 Uiso 1 1 calc R . .
C22 C 0.0057(3) 0.6474(3) 0.54909(19) 0.0457(6) Uani 1 1 d
H22 H -0.0747 0.5895 0.5246 0.055 Uiso 1 1 calc R . .
F22 F -0.0343(3) 0.7167(2) 0.63204(15) 0.0813(7) Uani 1 1 d
C23 C 0.0263(3) 0.7279(3) 0.4558(2) 0.0454(6) Uani 1 1 d
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H23B H -0.0678 0.7667 0.4274 0.055 Uiso 1 1 calc R . .
C24 C 0.0802(3) 0.6567(2) 0.36680(17) 0.0343(5) Uani 1 1 d
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O24 O 0.0924(2) 0.73027(16) 0.27580(13) 0.0433(4) Uani 1 1 d
H24A H 0.1676 0.7726 0.2891 0.065 Uiso 1 1 calc R . .
C25 C 0.2241(3) 0.5945(3) 0.41084(18) 0.0416(5) Uani 1 1 d
H25A H 0.2997 0.6547 0.4362 0.050 Uiso 1 1 calc R . .
H25B H 0.2581 0.5476 0.3536 0.050 Uiso 1 1 calc R . .
C26 C 0.2027(3) 0.5119(2) 0.50336(19) 0.0473(6) Uani 1 1 d
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O21 O 0.1076(2) 0.49112(17) 0.66804(12) 0.0491(5) Uani 1 1 d
C27 C 0.1473(2) 0.5112(2) 0.77443(16) 0.0333(4) Uani 1 1 d
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H212 H 0.1544 0.3546 1.2370 0.058 Uiso 1 1 calc R . .

S12

C213 C 0.1720(3) 0.4809(3) 1.12349(19) 0.0468(6) Uani 1 1 d . . .
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S13

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into account individually in the estimation of esds in distances,
angles
and torsion angles; correlations between esds in cell parameters are
only
used when they are defined by crystal symmetry. An approximate
(isotropic)
treatment of cell esds is used for estimating esds involving l.s.
planes.
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S14

C212 C213 1.386(4) . . ?

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S16

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S17

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_cell_angle_beta                93.54(2)
_cell_angle_gamma                90.00
_cell_volume                    2552.9(11)
_cell_formula_units_Z            8
_cell_measurement_temperature    223(2)
_cell_measurement_reflns_used    25
_cell_measurement_theta_min      40.20
_cell_measurement_theta_max      46.79

_exptl_crystal_description      'block'
_exptl_crystal_colour            'colourless'
_exptl_crystal_size_max         0.30
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_exptl_crystal_size_min          0.15
_exptl_crystal_density_meas      ?
_exptl_crystal_density_diffrn    1.318
_exptl_crystal_density_method    'not measured'
_exptl_crystal_F_000             1072
_exptl_absorpt_coefficient_mu     0.866
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_exptl_absorpt_correction_T_min  0.7813
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_diffrn_ambient_temperature      223(2)
_diffrn_radiation_wavelength     1.54178
_diffrn_radiation_type           CuK\alpha
_diffrn_radiation_source         'fine-focus sealed tube'
_diffrn_radiation_monochromator   graphite
_diffrn_measurement_device_type   'Enraf Nonius CAD4'
_diffrn_measurement_method       '\w/2q scans'
_diffrn_detector_area_resol_mean ?
_diffrn_standards_number         3
_diffrn_standards_interval_count 250
_diffrn_standards_interval_time  120
_diffrn_standards_decay_%       0.9
_diffrn_reflns_number            5310
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_diffrn_reflns_av_sigmaI/netI    0.0321
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_diffrn_reflns_limit_h_max       10
_diffrn_reflns_limit_k_min       0
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_diffrn_reflns_limit_l_min       0
_diffrn_reflns_limit_l_max       28
_diffrn_reflns_theta_min         3.88
_diffrn_reflns_theta_max         74.20
_reflns_number_total             5182
_reflns_number_gt                3941
_reflns_threshold_expression      >2sigma(I)

_computing_data_collection        'Express (Nonius B.V., 1994)'
_computing_cell_refinement        'Express (Nonius B.V., 1994)'
_computing_data_reduction         'MOLLEN (Fair, 1990)'
_computing_structure_solution     'SHELXS-97 (Sheldrick, 1990)'
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_computing_molecular_graphics     'Diamond (Brandenburg, 1997)'
_computing_publication_material   'SHELXL-97 (Sheldrick, 1997)'

_refine_special_details
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Refinement of F2 against ALL reflections. The weighted R-factor
wR and
goodness of fit S are based on F2, conventional R-factors R are
based
```

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on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > 2\sigma(F^2)$ 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.

The fluorine atom is disordered over the C2 and C6 positions (0.85(1) to 0.15/ 0.53(1) to 0.47 for the C22 and C26 positions).

```
;
_refine_ls_structure_factor_coef  Fsqd
_refine_ls_matrix_type            full
_refine_ls_weighting_scheme
'calc w=1/[\s^2^(Fo^2)+(0.0711P)^2+0.6319P] where
P=(Fo^2+2Fc^2)/3'
_atom_sites_solution_primary      direct
_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    'at N's from difmap, others geom'
_refine_ls_hydrogen_treatment     'refined as riding atoms'
_refine_ls_extinction_method       SHELXL
_refine_ls_extinction_coef        0.0021(2)
_refine_ls_extinction_expression
'Fc^*=kFc[1+0.001xFc^2\l^3^/sin(2\q)]^-1/4^'
_refine_ls_number_reflns          5182
_refine_ls_number_parameters      354
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_refine_ls_wR_factor_ref          0.1422
_refine_ls_wR_factor_gt          0.1306
_refine_ls_goodness_of_fit_ref    1.073
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_refine_ls_shift/su_mean          0.000

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  _atom_site_fract_z
  _atom_site_U_iso_or_equiv
  _atom_site_adp_type
  _atom_site_occupancy
  _atom_site_calc_flag
  _atom_site_refinement_flags
  _atom_site_disorder_assembly
  _atom_site_disorder_group
O1 O 0.99075(18) 0.15317(11) 0.17861(6) 0.0553(4) Uani 1 d . . .
C1 C 1.0105(2) 0.23428(15) 0.22291(8) 0.0451(4) Uani 1 d . . .
H1 H 0.9439 0.2195 0.2554 0.054 Uiso 1 calc R A 1
C2A C 0.9603(2) 0.33462(16) 0.19246(9) 0.0499(5) Uani 0.846(4) d P B
1
```

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H2A H 1.0180 0.3434 0.1569 0.060 Uiso 0.846(4) calc PR B 1
F2 F 0.80523(17) 0.32794(13) 0.17582(7) 0.0674(6) Uani 0.846(4) d P B
1
C2B C 0.9603(2) 0.33462(16) 0.19246(9) 0.0499(5) Uani 0.154(4) d P B
2
H2B1 H 0.8516 0.3296 0.1803 0.060 Uiso 0.154(4) calc PR B 2
H2B2 H 1.0167 0.3433 0.1571 0.060 Uiso 0.154(4) calc PR B 2
C3 C 0.9862(3) 0.43005(17) 0.23134(10) 0.0605(6) Uani 1 d . . .
H3A H 0.9614 0.4935 0.2085 0.073 Uiso 1 calc R C 1
H3B H 0.9175 0.4268 0.2635 0.073 Uiso 1 calc R C 1
C4 C 1.1494(3) 0.43704(17) 0.25657(9) 0.0553(5) Uani 1 d . . .
H4 H 1.1588 0.4959 0.2849 0.066 Uiso 1 calc R . .
O4 O 1.2446(2) 0.45694(15) 0.20883(6) 0.0704(5) Uani 1 d . . .
H4A H 1.3289 0.4789 0.2220 0.106 Uiso 1 calc R . .
C5 C 1.1949(2) 0.33548(17) 0.28754(9) 0.0523(5) Uani 1 d . . .
H5A H 1.1325 0.3257 0.3212 0.063 Uiso 1 calc R D 1
H5B H 1.3019 0.3398 0.3023 0.063 Uiso 1 calc R D 1
C6A C 1.1741(2) 0.24193(17) 0.24666(9) 0.0512(5) Uani 0.154(4) d P B
1
H6A H 1.2333 0.2590 0.2124 0.061 Uiso 0.154(4) calc PR B 1
F6 F 1.2314(14) 0.1619(9) 0.2673(6) 0.103(5) Uani 0.154(4) d P B 1
C6B C 1.1741(2) 0.24193(17) 0.24666(9) 0.0512(5) Uani 0.846(4) d P B
2
H6B1 H 1.2409 0.2495 0.2141 0.061 Uiso 0.846(4) calc PR B 2
H6B2 H 1.2029 0.1775 0.2680 0.061 Uiso 0.846(4) calc PR B 2
C7 C 0.9640(2) 0.05519(15) 0.19695(8) 0.0451(4) Uani 1 d . . .
O7 O 0.96382(19) 0.02912(11) 0.24803(6) 0.0582(4) Uani 1 d . . .
N8 N 0.9393(2) -0.00835(13) 0.14991(7) 0.0467(4) Uani 1 d . . .
H8 H 0.947(3) 0.0226(18) 0.1179(10) 0.056 Uiso 1 d . . .
C8 C 0.8874(2) -0.11336(14) 0.14933(8) 0.0423(4) Uani 1 d . . .
C9 C 0.8867(2) -0.17672(16) 0.19855(9) 0.0510(5) Uani 1 d . . .
H9 H 0.9229 -0.1508 0.2353 0.061 Uiso 1 calc R . .
C10 C 0.8324(3) -0.27852(17) 0.19331(11) 0.0598(6) Uani 1 d . . .
H10 H 0.8337 -0.3216 0.2267 0.072 Uiso 1 calc R . .
C11 C 0.7771(3) -0.31752(18) 0.14048(12) 0.0685(7) Uani 1 d . . .
H11 H 0.7391 -0.3864 0.1376 0.082 Uiso 1 calc R . .
C12 C 0.7779(3) -0.25443(18) 0.09140(11) 0.0684(6) Uani 1 d . . .
H12 H 0.7396 -0.2804 0.0549 0.082 Uiso 1 calc R . .
C13 C 0.8343(3) -0.15338(16) 0.09549(9) 0.0536(5) Uani 1 d . . .
H13 H 0.8368 -0.1116 0.0616 0.064 Uiso 1 calc R . .
O21 O 0.92679(14) 0.28864(10) 0.03400(6) 0.0480(3) Uani 1 d . . .
C21 C 0.7696(2) 0.27598(16) 0.01204(9) 0.0500(5) Uani 1 d . . .
H21 H 0.7245 0.2129 0.0294 0.060 Uiso 1 calc R E 1
C22A C 0.6888(2) 0.37419(18) 0.03140(10) 0.0565(5) Uani 0.527(4) d P
F 1
H22A H 0.6993 0.3819 0.0746 0.068 Uiso 0.527(4) calc PR F 1
F22 F 0.5341(3) 0.3510(2) 0.01215(14) 0.0846(12) Uani 0.527(4) d P F
1
C22B C 0.6888(2) 0.37419(18) 0.03140(10) 0.0565(5) Uani 0.473(4) d P
F 2
H22B H 0.5788 0.3662 0.0226 0.068 Uiso 0.473(4) calc PR F 2
H22C H 0.7063 0.3822 0.0739 0.068 Uiso 0.473(4) calc PR F 2
C23 C 0.7429(2) 0.47222(16) 0.00152(9) 0.0511(5) Uani 1 d . . .
H23A H 0.6808 0.5321 0.0126 0.061 Uiso 1 calc R G 1
H23B H 0.8490 0.4865 0.0149 0.061 Uiso 1 calc R G 1
C24 C 0.7319(2) 0.46066(14) -0.06449(8) 0.0462(4) Uani 1 d . . .
H24 H 0.6233 0.4527 -0.0782 0.055 Uiso 1 calc R . .
O24 O 0.7907(2) 0.55376(11) -0.08922(6) 0.0600(4) Uani 1 d . . .

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H24A H 0.7798 0.5506 -0.1255 0.090 Uiso 1 calc R . .
C25 C 0.8191(3) 0.36505(15) -0.08265(9) 0.0516(5) Uani 1 d . . .
H25A H 0.8069 0.3572 -0.1254 0.062 Uiso 1 calc R H 1
H25B H 0.9279 0.3750 -0.0719 0.062 Uiso 1 calc R H 1
C26A C 0.7645(2) 0.26674(15) -0.05397(10) 0.0534(5) Uani 0.473(4) d P
F 1
H26A H 0.8221 0.2046 -0.0662 0.064 Uiso 0.473(4) calc PR F 1
F26 F 0.6029(3) 0.2543(2) -0.06830(14) 0.0744(11) Uani 0.473(4) d P F
1
C26B C 0.7645(2) 0.26674(15) -0.05397(10) 0.0534(5) Uani 0.527(4) d P
F 2
H26B H 0.8284 0.2076 -0.0647 0.064 Uiso 0.527(4) calc PR F 2
H26C H 0.6595 0.2520 -0.0687 0.064 Uiso 0.527(4) calc PR F 2
C27 C 1.0101(2) 0.20079(14) 0.04478(7) 0.0388(4) Uani 1 d . . .
O27 O 0.95897(15) 0.11228(10) 0.03985(6) 0.0467(3) Uani 1 d . . .
N28 N 1.15403(17) 0.22959(12) 0.06102(7) 0.0417(4) Uani 1 d . . .
H28 H 1.177(2) 0.2959(18) 0.0643(9) 0.050 Uiso 1 d . . .
C28 C 1.2783(2) 0.16297(14) 0.07731(8) 0.0394(4) Uani 1 d . . .
C29 C 1.2852(2) 0.05824(15) 0.06143(9) 0.0502(5) Uani 1 d . . .
H29 H 1.2027 0.0264 0.0401 0.060 Uiso 1 calc R . .
C210 C 1.4159(3) 0.00103(17) 0.07755(11) 0.0613(6) Uani 1 d . . .
H210 H 1.4220 -0.0697 0.0664 0.074 Uiso 1 calc R . .
C211 C 1.5359(3) 0.04599(19) 0.10945(11) 0.0644(6) Uani 1 d . . .
H211 H 1.6228 0.0059 0.1205 0.077 Uiso 1 calc R . .
C212 C 1.5291(2) 0.14971(19) 0.12523(10) 0.0583(5) Uani 1 d . . .
H212 H 1.6115 0.1807 0.1470 0.070 Uiso 1 calc R . .
C213 C 1.4010(2) 0.20866(16) 0.10905(9) 0.0476(4) Uani 1 d . . .
H213 H 1.3970 0.2799 0.1196 0.057 Uiso 1 calc R . .

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_atom_site_aniso_U_23
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_atom_site_aniso_U_12
O1 0.0818(10) 0.0418(7) 0.0418(7) -0.0013(6) 0.0005(7) -0.0152(7)
C1 0.0542(11) 0.0413(10) 0.0393(9) -0.0029(7) 0.0005(8) -0.0075(8)
C2A 0.0517(11) 0.0489(11) 0.0479(11) 0.0018(9) -0.0076(8) -0.0050(9)
F2 0.0532(9) 0.0798(12) 0.0667(10) 0.0089(8) -0.0172(7) -0.0036(7)
C2B 0.0517(11) 0.0489(11) 0.0479(11) 0.0018(9) -0.0076(8) -0.0050(9)
C3 0.0706(14) 0.0459(12) 0.0636(13) -0.0014(10) -0.0075(11)
0.0037(10)
C4 0.0735(14) 0.0470(11) 0.0444(10) -0.0049(8) -0.0042(9) -0.0118(10)
O4 0.0851(12) 0.0802(11) 0.0448(8) 0.0049(7) -0.0055(7) -0.0371(9)
C5 0.0558(11) 0.0578(12) 0.0422(10) 0.0007(9) -0.0067(8) -0.0090(9)
C6A 0.0538(11) 0.0484(11) 0.0506(11) 0.0007(9) -0.0032(9) 0.0027(9)
F6 0.100(8) 0.078(8) 0.128(10) -0.048(7) -0.017(7) 0.019(6)
C6B 0.0538(11) 0.0484(11) 0.0506(11) 0.0007(9) -0.0032(9) 0.0027(9)
C7 0.0482(10) 0.0405(10) 0.0464(10) 0.0053(8) 0.0002(8) -0.0027(8)
O7 0.0794(10) 0.0497(8) 0.0452(8) 0.0055(6) 0.0010(7) -0.0028(7)
N8 0.0593(10) 0.0380(8) 0.0420(8) 0.0052(7) -0.0020(7) -0.0050(7)
C8 0.0373(9) 0.0378(9) 0.0520(10) 0.0012(8) 0.0035(7) 0.0035(7)
C9 0.0540(11) 0.0449(11) 0.0542(12) 0.0047(9) 0.0033(9) -0.0004(9)
C10 0.0658(13) 0.0441(11) 0.0712(14) 0.0082(10) 0.0190(11) 0.0001(10)
C11 0.0814(17) 0.0413(12) 0.0851(17) -0.0061(11) 0.0231(13) -
0.0095(11)

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C12 0.0853(17) 0.0507(13) 0.0692(15) -0.0149(11) 0.0053(13) -
0.0070(11)
C13 0.0643(13) 0.0442(11) 0.0522(11) -0.0032(9) 0.0035(9) 0.0009(9)
O21 0.0452(7) 0.0368(7) 0.0600(8) 0.0049(6) -0.0132(6) 0.0041(5)
C21 0.0419(10) 0.0462(10) 0.0604(12) 0.0153(9) -0.0077(8) -0.0015(8)
C22A 0.0497(11) 0.0660(14) 0.0539(12) 0.0153(10) 0.0036(9) 0.0118(10)
F22 0.0460(14) 0.099(2) 0.110(2) 0.0489(18) 0.0159(13) 0.0145(13)
C22B 0.0497(11) 0.0660(14) 0.0539(12) 0.0153(10) 0.0036(9) 0.0118(10)
C23 0.0566(11) 0.0479(11) 0.0483(10) -0.0007(9) -0.0008(9) 0.0136(9)
C24 0.0552(11) 0.0374(9) 0.0448(10) 0.0047(8) -0.0076(8) -0.0034(8)
O24 0.0933(11) 0.0375(7) 0.0483(8) 0.0043(6) -0.0037(8) -0.0118(7)
C25 0.0679(13) 0.0425(11) 0.0435(10) -0.0032(8) -0.0037(9) -0.0031(9)
C26A 0.0573(12) 0.0377(10) 0.0627(13) 0.0016(9) -0.0154(10) -
0.0041(8)
F26 0.0685(19) 0.0520(17) 0.098(2) 0.0016(14) -0.0345(15) -0.0143(13)
C26B 0.0573(12) 0.0377(10) 0.0627(13) 0.0016(9) -0.0154(10) -
0.0041(8)
C27 0.0438(9) 0.0362(9) 0.0358(8) 0.0034(7) -0.0035(7) 0.0034(7)
O27 0.0496(7) 0.0369(7) 0.0520(8) 0.0033(6) -0.0088(6) -0.0034(6)
N28 0.0437(8) 0.0308(7) 0.0495(9) 0.0023(6) -0.0064(6) 0.0013(6)
C28 0.0408(9) 0.0376(9) 0.0396(9) 0.0070(7) 0.0010(7) 0.0016(7)
C29 0.0513(11) 0.0383(10) 0.0603(12) 0.0019(9) -0.0032(9) 0.0034(8)
C210 0.0580(13) 0.0420(11) 0.0837(16) 0.0092(11) 0.0028(11) 0.0103(9)
C211 0.0451(11) 0.0622(14) 0.0853(16) 0.0211(12) -0.0005(11)
0.0133(10)
C212 0.0412(10) 0.0661(14) 0.0664(13) 0.0095(11) -0.0057(9) -
0.0010(9)
C213 0.0441(10) 0.0452(10) 0.0530(11) 0.0023(9) -0.0008(8) -0.0008(8)

_geom_special_details

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

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O1 C7 1.343(2) . ?

O1 C1 1.450(2) . ?

C1 C6A 1.508(3) . ?

C1 C2A 1.509(3) . ?

C2A F2 1.394(2) . ?

C2A C3 1.515(3) . ?

C3 C4 1.514(3) . ?

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C4 O4 1.438(3) . ?
C4 C5 1.517(3) . ?
C5 C6A 1.519(3) . ?
C6A F6 1.219(12) . ?
C7 O7 1.214(2) . ?
C7 N8 1.353(3) . ?
N8 C8 1.414(2) . ?
C8 C9 1.385(3) . ?
C8 C13 1.386(3) . ?
C9 C10 1.385(3) . ?
C10 C11 1.367(4) . ?
C11 C12 1.380(4) . ?
C12 C13 1.381(3) . ?
O21 C27 1.352(2) . ?
O21 C21 1.449(2) . ?
C21 C26A 1.511(3) . ?
C21 C22A 1.518(3) . ?
C22A F22 1.432(3) . ?
C22A C23 1.514(3) . ?
C23 C24 1.512(3) . ?
C24 O24 1.425(2) . ?
C24 C25 1.511(3) . ?
C25 C26A 1.506(3) . ?
C26A F26 1.445(3) . ?
C27 O27 1.217(2) . ?
C27 N28 1.346(2) . ?
N28 C28 1.414(2) . ?
C28 C29 1.386(3) . ?
C28 C213 1.389(3) . ?
C29 C210 1.391(3) . ?
C210 C211 1.370(3) . ?
C211 C212 1.373(3) . ?
C212 C213 1.384(3) . ?

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C7 O1 C1 117.46(15) . . ?
O1 C1 C6A 111.56(17) . . ?
O1 C1 C2A 105.29(15) . . ?
C6A C1 C2A 110.85(16) . . ?
F2 C2A C1 109.07(17) . . ?
F2 C2A C3 108.54(18) . . ?
C1 C2A C3 112.41(16) . . ?
C4 C3 C2A 112.02(19) . . ?
O4 C4 C3 107.64(17) . . ?
O4 C4 C5 110.83(19) . . ?
C3 C4 C5 110.08(17) . . ?
C4 C5 C6A 111.40(16) . . ?
F6 C6A C1 116.5(6) . . ?
F6 C6A C5 112.8(5) . . ?
C1 C6A C5 110.34(17) . . ?
O7 C7 O1 124.44(18) . . ?

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O7 C7 N8 126.20(18) . . ?
O1 C7 N8 109.36(16) . . ?
C7 N8 C8 127.59(17) . . ?
C9 C8 C13 119.22(19) . . ?
C9 C8 N8 124.21(18) . . ?
C13 C8 N8 116.57(17) . . ?
C10 C9 C8 119.7(2) . . ?
C11 C10 C9 121.2(2) . . ?
C10 C11 C12 119.1(2) . . ?
C11 C12 C13 120.5(2) . . ?
C12 C13 C8 120.2(2) . . ?
C27 O21 C21 117.68(14) . . ?
O21 C21 C26A 108.86(16) . . ?
O21 C21 C22A 105.07(16) . . ?
C26A C21 C22A 111.68(16) . . ?
F22 C22A C23 110.49(18) . . ?
F22 C22A C21 101.0(2) . . ?
C23 C22A C21 112.57(17) . . ?
C24 C23 C22A 111.50(18) . . ?
O24 C24 C25 111.12(17) . . ?
O24 C24 C23 108.17(15) . . ?
C25 C24 C23 110.49(16) . . ?
C26A C25 C24 111.77(18) . . ?
F26 C26A C25 109.11(19) . . ?
F26 C26A C21 101.7(2) . . ?
C25 C26A C21 112.27(16) . . ?
O27 C27 N28 127.82(16) . . ?
O27 C27 O21 123.94(16) . . ?
N28 C27 O21 108.24(15) . . ?
C27 N28 C28 127.23(15) . . ?
C29 C28 C213 119.70(17) . . ?
C29 C28 N28 123.70(17) . . ?
C213 C28 N28 116.55(16) . . ?
C28 C29 C210 119.0(2) . . ?
C211 C210 C29 121.2(2) . . ?
C210 C211 C212 119.9(2) . . ?
C211 C212 C213 120.0(2) . . ?
C212 C213 C28 120.25(19) . . ?

_diffirn_measured_fraction_theta_max	0.955
_diffirn_reflns_theta_full	74.20
_diffirn_measured_fraction_theta_full	0.955
_refine_diff_density_max	0.217
_refine_diff_density_min	-0.234
_refine_diff_density_rms	0.047