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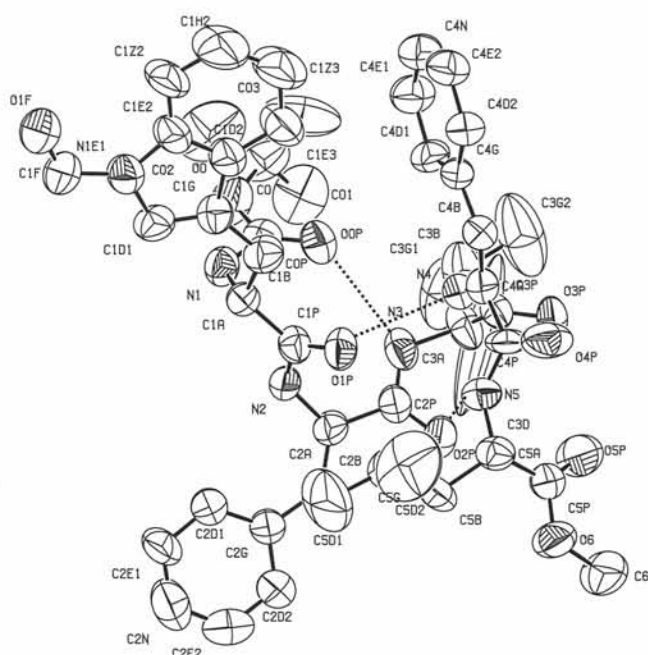
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Crystal structure of Boc-Trp(CHO)- Δ Phe-Ile- Δ Phe-Leu-OCH₃, C₄₈H₅₉N₆O₁₀

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Abstract

C₄₈H₅₉N₆O₁₀, orthorhombic, *P*2₁2₁2₁ (No. 19), *a* = 19.276(5) Å, *b* = 19.439(5) Å, *c* = 13.352(5) Å, *V* = 5003.1 Å³, *Z* = 4, *R*_{gt}(*F*) = 0.077, *wR*_{ref}(*F*²) = 0.230, *T* = 293 K.

Source of material

The title peptide has been synthesised using the mixed anhydride coupling and the azalactone method according to [1] and [2] respectively. The peptide was crystallised from its solution in acetone-water mixture (4:1) by slow evaporation method.

Experimental details

The ratio *N*(*hkl*)_{obs}/*N*(*param*) is relative low (4.8) which is a result of the relative low crystal quality. The side chains of Ile and Leu are thermally disordered. The atoms C3D and C5D1 were refined isotropically.

Discussion

The specific folded structures can be generated with α,β -dehydro-residues. A set of design rules have been developed with dehydro-residues [3]. However, there have been still some gaps in finalizing some of these rules. In order to generalize the design rules, a new pentapeptide sequence was synthesized with two

Δ Phe residues at (*i*+2) and (*i*+4) positions. The remaining three positions in the pentapeptide are filled with high constraint generating residues such as Trp, Ile and Leu. This is the first sequence with Trp at (*i*+1) position and two Δ Phe residues are separated by a branched β -carbon residue Ile. In the peptide Boc-Trp(CHO)- Δ Phe-Ile- Δ Phe-Leu-OCH₃ the backbone torsion angles $\varphi_1 = -52.3(8)^\circ$, $\psi_1 = -49.1(7)^\circ$, $\omega_1 = -177.5(6)^\circ$, $\varphi_2 = -56.5(8)^\circ$, $\psi_2 = -31.4(9)^\circ$, $\omega_2 = 179.7(6)^\circ$, $\varphi_3 = -69.8(8)^\circ$, $\psi_3 = -31.3(9)^\circ$, $\omega_3 = 169.9(6)^\circ$, $\varphi_4 = -60.3(8)^\circ$, $\psi_4 = -28.4(9)^\circ$, $\omega_4 = -177.0(6)^\circ$, $\varphi_5 = -90.2(8)^\circ$, $\psi_5^T = 13(1)^\circ$ indicate that the peptide adopts a 3₁₀-helical conformation. The structure is stabilized by three N(*i*+3) → O=C(*i*) hydrogen bonds. The side chain torsion angles of Δ Phe₂ and Δ Phe₄ are $\chi_2^1 = -8(1)^\circ$, $\chi_2^{2,1} = -175(1)^\circ$, $\chi_2^{2,2} = 3(1)^\circ$ and $\chi_4^1 = -3(1)^\circ$, $\chi_4^{2,1} = -175.8(7)^\circ$, $\chi_4^{2,2} = 1(1)^\circ$ respectively and indicate that the side chain conformation of two Δ Phe residues are planar. The side chain conformation of sandwiched branched β -carbon residue Ile is found to be favourably staggered to the backbone with torsion angles $\chi_3^1 = -67.7(9)^\circ$, $\chi_3^{1,2} = 167(1)^\circ$, $\chi_3^2 = -64(2)^\circ$. It is noteworthy that the side chain conformation of isoleucine in the structure of Boc-Leu- Δ Phe-Ile- Δ Phe-Ile-OCH₃ [4] was not observed in the staggered arrangement thus causing considerable deviations from the planarity in the side chains of neighbouring Δ Phe residues. The side chain conformation of the leucyl residue with torsion angles $\chi_5^1 = -64.7(8)^\circ$, $\chi_5^{2,1} = 165(1)^\circ$ and $\chi_5^{2,2} = -61(1)^\circ$ is one of the most commonly observed conformations for the side chain of leucine [2]. Overall, the 3₁₀-helical conformation of the present peptide has all the side chains favourably aligned. Therefore, it can be stated that the structures of peptides with two Δ Phe residues at alternate positions will always result in the formation of a 3₁₀-helical conformation. In the crystal structure, the molecules are linked through two intermolecular hydrogen bonds *d*(N1–H1...O5P) = 2.898(8) Å and *d*(N2–H2...O7) = 2.98(1) Å.

Table 1. Data collection and handling.

| | |
|---|--|
| Crystal: | colorless prism, size 0.3 × 0.4 × 0.5 mm |
| Wavelength: | Cu K α radiation (1.54180 Å) |
| μ : | 6.74 cm ⁻¹ |
| Diffractometer, scan mode: | Enraf Nonius CAD4, $\omega/2\theta$ |
| $2\theta_{\max}$: | 139.96° |
| <i>N</i> (<i>hkl</i>) _{measured} , <i>N</i> (<i>hkl</i>) _{unique} : | 4783, 4745 |
| Criterion for <i>I</i> _{obs} , <i>N</i> (<i>hkl</i>) _{gt} : | <i>I</i> _{obs} > 2 σ (<i>I</i> _{obs}), 2762 |
| <i>N</i> (<i>param</i>) _{refined} : | 574 |
| Programs: | SHELXS-97 [5] SHELXL-97 [6] |

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Table 2. Atomic coordinates and displacement parameters (in Å²).

| Atom | Site | x | y | z | U _{iso} |
|--------|------|---------|---------|--------|------------------|
| H(01A) | 4a | 0.6143 | 0.5507 | 0.7866 | 0.08 |
| H(01B) | 4a | 0.6128 | 0.4863 | 0.7160 | 0.08 |
| H(01C) | 4a | 0.5598 | 0.4922 | 0.8046 | 0.08 |
| H(02A) | 4a | 0.4558 | 0.5214 | 0.5987 | 0.08 |
| H(02B) | 4a | 0.4640 | 0.4759 | 0.6948 | 0.08 |
| H(02C) | 4a | 0.5158 | 0.4671 | 0.6052 | 0.08 |
| H(03A) | 4a | 0.5377 | 0.6213 | 0.5724 | 0.08 |
| H(03B) | 4a | 0.6024 | 0.5725 | 0.5734 | 0.08 |
| H(03C) | 4a | 0.5976 | 0.6336 | 0.6498 | 0.08 |
| H(1) | 4a | 0.4106 | 0.6568 | 0.8400 | 0.08 |
| H(1A) | 4a | 0.4107 | 0.7529 | 0.9246 | 0.08 |
| H(1BA) | 4a | 0.4742 | 0.8441 | 0.8527 | 0.08 |
| H(1BB) | 4a | 0.5094 | 0.7918 | 0.7797 | 0.08 |
| H(1DA) | 4a | 0.3232 | 0.7795 | 0.8054 | 0.08 |
| H(1ZA) | 4a | 0.3041 | 0.8808 | 0.4751 | 0.08 |
| H(1HA) | 4a | 0.4021 | 0.9237 | 0.3971 | 0.08 |
| H(1EA) | 4a | 0.5228 | 0.8701 | 0.6281 | 0.08 |
| H(1F) | 4a | -0.0016 | -0.0013 | 0.0032 | 0.08 |
| H(2) | 4a | 0.4815 | 0.6609 | 1.0369 | 0.08 |
| H(2B) | 4a | 0.5854 | 0.6882 | 1.2563 | 0.08 |
| H(2DB) | 4a | 0.5300 | 0.6950 | 1.4076 | 0.08 |
| H(2DA) | 4a | 0.4084 | 0.6997 | 1.1639 | 0.08 |
| H(2EA) | 4a | 0.3143 | 0.6983 | 1.2649 | 0.08 |
| H(2EB) | 4a | 0.4327 | 0.7084 | 1.5029 | 0.08 |
| H(2NA) | 4a | 0.3241 | 0.7049 | 1.4328 | 0.08 |
| H(3) | 4a | 0.6232 | 0.6488 | 0.9664 | 0.08 |
| H(3A) | 4a | 0.7556 | 0.6625 | 1.0267 | 0.08 |
| H(3B) | 4a | 0.7036 | 0.6285 | 0.8343 | 0.08 |

Table 2. Continued.

| Atom | Site | x | y | z | U _{iso} |
|--------|------|-----------|-----------|-----------|------------------|
| H(3GA) | 4a | 0.8149 | 0.6019 | 0.7805 | 0.08 |
| H(3GB) | 4a | 0.8455 | 0.6326 | 0.8796 | 0.08 |
| H(3GC) | 4a | 0.8078 | 0.6807 | 0.8028 | 0.08 |
| H(3GD) | 4a | 0.6891 | 0.5443 | 0.9485 | 0.08 |
| H(3GE) | 4a | 0.7411 | 0.5201 | 0.8661 | 0.08 |
| C(3D) | 4a | 0.784(2) | 0.530(2) | 1.000(2) | 0.27(1) |
| H(4) | 4a | 0.6558 | 0.7688 | 0.8816 | 0.08 |
| H(4B) | 4a | 0.7024 | 0.9399 | 0.7973 | 0.08 |
| H(4DA) | 4a | 0.6669 | 0.7643 | 0.7228 | 0.08 |
| H(4DB) | 4a | 0.6874 | 0.9607 | 0.6354 | 0.08 |
| H(4EA) | 4a | 0.6474 | 0.7337 | 0.5557 | 0.08 |
| H(4EB) | 4a | 0.6696 | 0.9298 | 0.4699 | 0.08 |
| H(4N) | 4a | 0.6454 | 0.8158 | 0.4301 | 0.08 |
| H(5) | 4a | 0.6686 | 0.8404 | 1.0577 | 0.08 |
| H(5A) | 4a | 0.6994 | 0.9631 | 1.1411 | 0.08 |
| H(5BA) | 4a | 0.6175 | 0.855 | 1.2225 | 0.08 |
| H(5BB) | 4a | 0.6312 | 0.9239 | 1.2801 | 0.08 |
| H(5GA) | 4a | 0.5647 | 0.918 | 1.0948 | 0.08 |
| C(5D1) | 4a | 0.4965(8) | 0.9061(9) | 1.214(1) | 0.176(5) |
| H(5DD) | 4a | 0.5279 | 1.0290 | 1.1213 | 0.08 |
| H(5DE) | 4a | 0.6091 | 1.0243 | 1.1162 | 0.08 |
| H(5DF) | 4a | 0.5719 | 1.0322 | 1.2200 | 0.08 |
| H(6A) | 4a | 0.8091 | 0.9142 | 1.4309 | 0.08 |
| H(6C) | 4a | 0.8577 | 0.9154 | 1.3368 | 0.08 |
| H(6D) | 4a | 0.8214 | 0.8467 | 1.3690 | 0.08 |
| HW(1) | 4a | 0.054(4) | -0.155(4) | -0.091(6) | 0.08 |
| HW(2) | 4a | -0.035(4) | 0.165(3) | 0.108(5) | 0.08 |

Table 3. Atomic coordinates and displacement parameters (in Å²).

| Atom | Site | x | y | z | U ₁₁ | U ₂₂ | U ₃₃ | U ₁₂ | U ₁₃ | U ₂₃ |
|--------|------|-----------|-----------|-----------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| C(01) | 4a | 0.5849(6) | 0.5174(5) | 0.755(1) | 0.143(9) | 0.096(6) | 0.16(1) | 0.024(6) | -0.006(8) | 0.005(7) |
| C(02) | 4a | 0.4885(8) | 0.4995(6) | 0.643(1) | 0.20(1) | 0.14(1) | 0.22(2) | 0.07(1) | -0.04(1) | -0.09(1) |
| C(03) | 4a | 0.5716(9) | 0.5993(6) | 0.6142(9) | 0.33(2) | 0.118(8) | 0.095(7) | 0.06(1) | 0.06(1) | -0.010(7) |
| C(0) | 4a | 0.5355(6) | 0.5530(5) | 0.6879(8) | 0.136(8) | 0.083(5) | 0.104(7) | 0.029(5) | -0.013(6) | -0.034(6) |
| O(0) | 4a | 0.4854(3) | 0.5937(3) | 0.7477(5) | 0.088(3) | 0.090(4) | 0.130(5) | 0.010(3) | -0.012(4) | -0.039(4) |
| C(0P) | 4a | 0.5057(4) | 0.6463(4) | 0.8044(6) | 0.067(4) | 0.072(4) | 0.076(5) | 0.006(3) | 0.005(4) | -0.001(4) |
| O(0P) | 4a | 0.5656(2) | 0.6657(3) | 0.8168(4) | 0.062(3) | 0.094(3) | 0.095(4) | 0.004(2) | 0.008(3) | 0.000(3) |
| N(1) | 4a | 0.4502(3) | 0.6769(3) | 0.8434(4) | 0.066(3) | 0.068(3) | 0.081(4) | -0.011(3) | -0.006(3) | -0.007(3) |
| C(1A) | 4a | 0.4553(3) | 0.7441(3) | 0.8918(5) | 0.053(3) | 0.071(4) | 0.068(4) | 0.004(3) | 0.000(3) | 0.006(3) |
| C(1B) | 4a | 0.4669(4) | 0.8016(4) | 0.8161(5) | 0.076(4) | 0.072(4) | 0.066(4) | -0.003(3) | -0.011(3) | 0.012(3) |
| C(1G) | 4a | 0.4107(3) | 0.8132(3) | 0.7420(5) | 0.066(4) | 0.064(4) | 0.070(4) | 0.001(3) | 0.002(3) | 0.011(3) |
| C(1D2) | 4a | 0.4208(4) | 0.8445(4) | 0.6463(6) | 0.064(4) | 0.111(6) | 0.080(5) | 0.005(4) | 0.005(4) | 0.006(5) |
| C(1D1) | 4a | 0.3438(4) | 0.8008(4) | 0.7506(5) | 0.075(4) | 0.093(5) | 0.056(4) | 0.007(4) | -0.011(3) | 0.011(4) |
| N(1E1) | 4a | 0.3080(3) | 0.8242(3) | 0.6651(5) | 0.063(3) | 0.095(4) | 0.074(4) | 0.006(3) | 0.007(3) | -0.003(3) |
| C(1E2) | 4a | 0.3574(4) | 0.8515(5) | 0.6012(6) | 0.062(4) | 0.125(6) | 0.071(5) | 0.020(4) | 0.011(4) | -0.005(5) |
| C(1Z2) | 4a | 0.3475(5) | 0.8788(7) | 0.5054(7) | 0.080(5) | 0.23(1) | 0.065(5) | 0.023(7) | 0.017(4) | 0.049(7) |
| C(1H2) | 4a | 0.4068(6) | 0.902(1) | 0.4591(9) | 0.114(8) | 0.36(2) | 0.086(7) | 0.06(1) | 0.001(7) | 0.10(1) |
| CZ(3) | 4a | 0.4735(7) | 0.897(1) | 0.4990(9) | 0.117(8) | 0.36(2) | 0.087(8) | 0.03(1) | 0.026(6) | 0.09(1) |
| C(1E3) | 4a | 0.4798(5) | 0.8703(6) | 0.5965(7) | 0.068(5) | 0.19(1) | 0.099(7) | 0.022(6) | 0.022(5) | 0.034(7) |
| C(1F) | 4a | 0.2356(4) | 0.8186(6) | 0.6552(8) | 0.066(5) | 0.171(9) | 0.099(7) | 0.016(5) | -0.012(5) | 0.009(7) |
| O(1F) | 4a | 0.2071(3) | 0.8430(4) | 0.5816(5) | 0.070(3) | 0.182(6) | 0.107(5) | 0.011(3) | -0.013(3) | 0.008(5) |
| C(1P) | 4a | 0.5111(3) | 0.7463(4) | 0.9730(5) | 0.046(3) | 0.075(4) | 0.084(5) | 0.003(3) | -0.001(3) | 0.003(4) |
| O(1P) | 4a | 0.5526(2) | 0.7938(2) | 0.9796(4) | 0.055(2) | 0.077(3) | 0.095(3) | -0.009(2) | -0.006(2) | 0.004(3) |
| N(2) | 4a | 0.5107(3) | 0.6942(3) | 1.0412(4) | 0.056(3) | 0.082(4) | 0.059(3) | -0.014(3) | -0.005(2) | 0.012(3) |
| C(2A) | 4a | 0.5602(3) | 0.6968(4) | 1.1197(5) | 0.064(3) | 0.075(4) | 0.059(4) | -0.010(3) | -0.011(3) | 0.016(3) |
| C(2B) | 4a | 0.5462(3) | 0.6938(4) | 1.2166(6) | 0.060(4) | 0.118(6) | 0.066(5) | -0.016(4) | -0.010(3) | 0.023(4) |
| C(2G) | 4a | 0.4824(3) | 0.6974(5) | 1.2734(5) | 0.057(3) | 0.122(6) | 0.066(5) | -0.012(4) | -0.005(3) | 0.019(4) |
| C(2D2) | 4a | 0.4868(5) | 0.6983(6) | 1.3767(7) | 0.077(5) | 0.19(1) | 0.080(6) | -0.008(6) | -0.003(5) | 0.007(7) |
| C(2D1) | 4a | 0.4144(4) | 0.6992(5) | 1.2330(6) | 0.069(4) | 0.166(9) | 0.066(5) | -0.009(5) | 0.000(4) | 0.013(5) |
| C(2E1) | 4a | 0.3582(4) | 0.7000(6) | 1.2937(7) | 0.063(4) | 0.20(1) | 0.088(6) | -0.006(5) | 0.010(4) | 0.031(7) |
| C(2E2) | 4a | 0.4283(6) | 0.7039(6) | 1.4338(7) | 0.117(8) | 0.19(1) | 0.063(5) | -0.006(7) | -0.003(5) | -0.015(6) |
| C(2N) | 4a | 0.3634(5) | 0.7032(7) | 1.3926(9) | 0.090(6) | 0.20(1) | 0.102(8) | -0.013(7) | 0.025(6) | 0.021(8) |

Table 3. Continued.

| Atom | Site | <i>x</i> | <i>y</i> | <i>z</i> | <i>U</i> ₁₁ | <i>U</i> ₂₂ | <i>U</i> ₃₃ | <i>U</i> ₁₂ | <i>U</i> ₁₃ | <i>U</i> ₂₃ |
|--------|------|-----------|-----------|-----------|------------------------|------------------------|------------------------|------------------------|------------------------|------------------------|
| C(2P) | 4a | 0.6349(3) | 0.6996(4) | 1.0876(6) | 0.056(3) | 0.096(5) | 0.075(5) | -0.009(4) | 0.005(3) | 0.013(4) |
| O(2P) | 4a | 0.6783(2) | 0.7279(3) | 1.1430(4) | 0.060(3) | 0.143(5) | 0.091(4) | -0.022(3) | -0.007(3) | 0.017(3) |
| N(3) | 4a | 0.6532(3) | 0.6704(3) | 1.0022(5) | 0.053(3) | 0.077(3) | 0.086(4) | -0.004(2) | 0.004(3) | 0.022(3) |
| C(3A) | 4a | 0.7265(3) | 0.6755(4) | 0.9696(7) | 0.055(3) | 0.088(5) | 0.107(6) | 0.011(3) | 0.015(4) | 0.030(5) |
| C(3B) | 4a | 0.7405(4) | 0.6227(5) | 0.884(1) | 0.069(5) | 0.092(6) | 0.18(1) | 0.010(4) | 0.015(6) | -0.029(7) |
| C(3G2) | 4a | 0.8082(6) | 0.6356(7) | 0.832(1) | 0.14(1) | 0.15(1) | 0.34(2) | -0.035(8) | 0.10(1) | -0.10(1) |
| C(3G1) | 4a | 0.7356(6) | 0.5510(6) | 0.923(1) | 0.110(8) | 0.121(9) | 0.26(2) | 0.014(6) | -0.04(1) | 0.00(1) |
| C(3P) | 4a | 0.7453(3) | 0.7496(4) | 0.9410(5) | 0.055(3) | 0.090(5) | 0.067(4) | -0.006(3) | 0.012(3) | -0.004(4) |
| O(3P) | 4a | 0.8036(2) | 0.7705(3) | 0.9548(4) | 0.047(2) | 0.106(4) | 0.098(3) | -0.009(2) | 0.001(2) | 0.005(3) |
| N(4) | 4a | 0.6941(2) | 0.7880(3) | 0.8993(4) | 0.054(3) | 0.082(4) | 0.057(3) | -0.007(3) | 0.002(2) | 0.005(3) |
| C(4A) | 4a | 0.7036(3) | 0.8591(4) | 0.8848(5) | 0.057(3) | 0.086(5) | 0.061(4) | -0.010(3) | -0.003(3) | 0.005(4) |
| C(4B) | 4a | 0.6957(3) | 0.8925(4) | 0.7943(5) | 0.059(3) | 0.088(4) | 0.062(4) | -0.001(3) | 0.005(3) | -0.004(4) |
| C(4G) | 4a | 0.6791(3) | 0.8672(4) | 0.6970(4) | 0.058(3) | 0.089(5) | 0.043(3) | -0.008(3) | -0.002(3) | 0.010(3) |
| C(4D1) | 4a | 0.6670(4) | 0.7977(4) | 0.6730(5) | 0.081(4) | 0.088(5) | 0.057(4) | -0.011(4) | -0.013(3) | 0.009(4) |
| C(4D2) | 4a | 0.6794(3) | 0.9147(4) | 0.6201(5) | 0.076(4) | 0.086(4) | 0.055(4) | -0.005(4) | -0.001(3) | 0.003(4) |
| C(4E1) | 4a | 0.6551(4) | 0.7796(4) | 0.5718(6) | 0.102(5) | 0.087(5) | 0.075(5) | -0.012(4) | 0.003(4) | -0.007(4) |
| C(4E2) | 4a | 0.6681(4) | 0.8965(5) | 0.5198(6) | 0.096(5) | 0.096(6) | 0.063(5) | -0.010(4) | 0.005(4) | 0.008(4) |
| C(4N) | 4a | 0.6546(5) | 0.8285(5) | 0.4959(6) | 0.112(6) | 0.112(6) | 0.053(4) | -0.003(5) | -0.002(4) | 0.018(4) |
| C(4P) | 4a | 0.7176(4) | 0.9023(4) | 0.9731(4) | 0.097(5) | 0.089(5) | 0.025(3) | -0.004(4) | 0.001(3) | 0.006(3) |
| O(4P) | 4a | 0.7488(4) | 0.9568(3) | 0.9705(4) | 0.169(6) | 0.110(4) | 0.068(3) | -0.066(4) | 0.012(4) | -0.006(3) |
| N(5) | 4a | 0.6903(3) | 0.8790(3) | 1.0594(4) | 0.080(3) | 0.068(3) | 0.061(3) | 0.000(3) | -0.002(3) | -0.002(3) |
| C(5A) | 4a | 0.6945(3) | 0.9138(4) | 1.1548(5) | 0.069(4) | 0.072(4) | 0.054(4) | 0.010(3) | 0.003(3) | 0.003(3) |
| C(5B) | 4a | 0.6260(3) | 0.9038(5) | 1.2140(6) | 0.067(4) | 0.125(6) | 0.064(4) | 0.013(4) | 0.017(3) | 0.018(4) |
| C(5G) | 4a | 0.5646(4) | 0.9358(6) | 1.1635(7) | 0.069(4) | 0.155(8) | 0.080(5) | 0.025(5) | -0.007(4) | -0.022(6) |
| C(5D2) | 4a | 0.5687(8) | 1.0121(7) | 1.154(1) | 0.17(1) | 0.18(1) | 0.28(2) | 0.10(1) | -0.06(1) | -0.01(1) |
| C(5P) | 4a | 0.7585(3) | 0.8910(4) | 1.2078(6) | 0.059(4) | 0.103(5) | 0.057(4) | -0.001(4) | 0.002(3) | -0.010(4) |
| O(5P) | 4a | 0.8053(3) | 0.8600(4) | 1.1751(5) | 0.083(4) | 0.180(6) | 0.093(4) | 0.041(4) | -0.011(3) | -0.034(4) |
| O(6) | 4a | 0.7582(3) | 0.9123(4) | 1.3027(4) | 0.078(3) | 0.173(6) | 0.069(4) | 0.036(4) | -0.012(3) | -0.025(4) |
| C(6) | 4a | 0.8164(5) | 0.8958(7) | 1.3650(7) | 0.090(6) | 0.18(1) | 0.091(6) | 0.042(6) | -0.023(5) | -0.004(6) |
| O(7) | 4a | 0.9009(4) | 0.9135(4) | 0.9662(8) | 0.136(5) | 0.168(7) | 0.193(8) | 0.081(5) | -0.003(6) | 0.015(7) |

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