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Atomic Coordinates and Displacement Parameters

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O3 C31 C36 C37 -3.0(4) . . . . no
C32 C31 C36 C37 174.4(2) . . . . no
C35 C36 C37 C42 61.0(3) . . . . no
C31 C36 C37 C42 -115.8(3) . . . . no
C348 O4 C41 C42 94.8(3) . . . . no
C348 O4 C41 C46 -88.6(3) . . . . no
O4 C41 C42 C43 177.8(2) . . . . no
C46 C41 C42 C43 1.3(4) . . . . no
O4 C41 C42 C37 1.0(4) . . . . no
C46 C41 C42 C37 -175.5(2) . . . . no
C36 C37 C42 C41 81.2(3) . . . . no
C36 C37 C42 C43 -95.5(3) . . . . no
C41 C42 C43 C44 -1.3(4) . . . . no
C37 C42 C43 C44 175.4(2) . . . . no

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C42 C43 C44 C45 0.1(4) no
C43 C44 C45 C46 1.1(4) no
C44 C45 C46 C41 -1.1(4) no
C44 C45 C46 C47 175.7(3) no
O4 C41 C46 C45 -176.6(2) no
C42 C41 C46 C45 -0.1(4) no
O4 C41 C46 C47 6.9(4) no
C42 C41 C46 C47 -176.6(3) no
C13 C12 C47 C46 149.4(3) no
C11 C12 C47 C46 -35.7(4) no
C45 C46 C47 C12 148.0(3) no
C41 C46 C47 C12 -35.5(4) no
C11 O1 C121 C122 176.4(2) no
O1 C121 C122 O123 171.9(2) no
C121 C122 O123 C124 -116.3(3) no
C122 O123 C124 C125 82.9(3) no
O123 C124 C125 O126 -69.6(3) no
C124 C125 O126 C127 -82.9(3) no
C125 O126 C127 C128 170.9(2) no
C21 O2 C128 C127 172.8(2) no
O126 C127 C128 O2 -67.1(3) no
C31 O3 C341 C342 178.3(2) no
O3 C341 C342 O343 -69.1(3) no
C341 C342 O343 C344 170.3(2) no
C342 O343 C344 C345 -83.0(3) no
O343 C344 C345 O346 -65.4(3) no
C344 C345 O346 C347 86.6(3) no
C345 O346 C347 C348 -122.7(3) no
C41 O4 C348 C347 173.6(2) no
O346 C347 C348 O4 173.6(2) no
C561 O5 C51 C52 90.3(3) no
C561 O5 C51 C56 -94.3(3) no
O5 C51 C52 C53 176.4(2) no
C56 C51 C52 C53 1.1(4) no
O5 C51 C52 C87 -6.2(4) no
C56 C51 C52 C87 178.5(2) no
C51 C52 C53 C54 0.0(4) no
C87 C52 C53 C54 -177.6(2) no
C52 C53 C54 C55 0.1(4) no
C53 C54 C55 C56 -1.2(4) no
C54 C55 C56 C51 2.2(4) no
C54 C55 C56 C57 -175.8(2) no
O5 C51 C56 C55 -177.6(2) no
C52 C51 C56 C55 -2.2(4) no
O5 C51 C56 C57 0.5(4) no
C52 C51 C56 C57 175.9(2) no
C55 C56 C57 C62 91.2(3) no
C51 C56 C57 C62 -86.8(3) no
C568 O6 C61 C66 -92.3(3) no
C568 O6 C61 C62 90.7(3) no
C66 C61 C62 C63 3.6(4) no
O6 C61 C62 C63 -179.5(2) no
C66 C61 C62 C57 -174.6(3) no
O6 C61 C62 C57 2.3(4) no
C56 C57 C62 C63 -61.8(3) no
C56 C57 C62 C61 116.3(3) no
C61 C62 C63 C64 -0.8(4) no
C57 C62 C63 C64 177.3(3) no
C62 C63 C64 C65 -1.5(4) no
C63 C64 C65 C66 1.2(4) no
C64 C65 C66 C61 1.4(4) no
C64 C65 C66 C67 -174.9(3) no
O6 C61 C66 C65 179.2(2) no
C62 C61 C66 C65 -3.9(4) no
O6 C61 C66 C67 -4.4(4) no
C62 C61 C66 C67 172.5(3) no
C65 C66 C67 C72 119.7(3) no
C61 C66 C67 C72 -56.6(4) no
C781 O7 C71 C76 96.3(3) no
C781 O7 C71 C72 -85.2(3) no
O7 C71 C72 C73 177.4(2) no
C76 C71 C72 C73 -4.2(4) no
O7 C71 C72 C67 -3.8(4) no

C76 C71 C72 C67 174.7(2) no
 C66 C67 C72 C73 131.1(3) no
 C66 C67 C72 C71 -47.7(4) no
 C71 C72 C73 C74 1.9(4) no
 C67 C72 C73 C74 -177.0(3) no
 C72 C73 C74 C75 1.2(4) no
 C73 C74 C75 C76 -2.1(4) no
 C74 C75 C76 C71 -0.2(4) no
 C74 C75 C76 C77 178.6(2) no
 O7 C71 C76 C75 -178.2(2) no
 C72 C71 C76 C75 3.4(4) no
 O7 C71 C76 C77 3.0(4) no
 C72 C71 C76 C77 -175.4(2) no
 C75 C76 C77 C82 -67.4(3) no
 C71 C76 C77 C82 111.4(3) no
 C788 O8 C81 C82 -99.6(3) no
 C788 O8 C81 C86 85.5(3) no
 O8 C81 C82 C83 -174.8(2) no
 C86 C81 C82 C83 -0.1(4) no
 O8 C81 C82 C77 0.9(4) no
 C86 C81 C82 C77 175.6(3) no
 C76 C77 C82 C81 -87.9(3) no
 C76 C77 C82 C83 87.7(3) no
 C81 C82 C83 C84 0.3(4) no
 C77 C82 C83 C84 -175.4(3) no
 C82 C83 C84 C85 -0.1(4) no
 C83 C84 C85 C86 -0.4(4) no
 C82 C81 C86 C85 -0.4(4) no
 O8 C81 C86 C85 174.3(2) no
 C82 C81 C86 C87 178.1(3) no
 O8 C81 C86 C87 -7.3(4) no
 C84 C85 C86 C81 0.6(4) no
 C84 C85 C86 C87 -177.9(3) no
 C51 C52 C87 C86 38.1(4) no
 C53 C52 C87 C86 -144.5(3) no
 C81 C86 C87 C52 35.0(4) no
 C85 C86 C87 C52 -146.5(3) no
 C51 O5 C561 C562 -174.3(2) no
 O5 C561 C562 O563 -174.0(2) no
 C561 C562 O563 C564 120.8(3) no
 C562 O563 C564 C565 -82.8(3) no
 O563 C564 C565 O566 65.7(3) no
 C564 C565 O566 C567 82.1(3) no
 C565 O566 C567 C568 -175.3(2) no
 C61 O6 C568 C567 -174.5(2) no
 O566 C567 C568 O6 70.5(3) no
 C71 O7 C781 C782 178.3(2) no
 O7 C781 C782 O783 73.2(3) no
 C781 C782 O783 C784 -175.8(2) no
 C782 O783 C784 C785 81.2(3) no
 O783 C784 C785 O786 64.8(3) no
 C784 C785 O786 C787 -86.7(3) no
 C785 O786 C787 C788 124.2(3) no
 C81 O8 C788 C787 -170.8(2) no
 O786 C787 C788 O8 -169.1(2) no

#=====

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 # END of CIF
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