SUPPLEMENTARY MATERIAL

X-ray crystallographic data for **1** (DS2 and DS3) and for **2** (DS5) in CIF format file are available free of charge from the Cambridge Crystallographic Data Centre *via* www.ccdc.cam.ac.uk/data_request/cif (deposition numbers, CCDC 745049 - 745051).

```
##############################################################################
# CIF Formatted file for the structures relevant the paper:                  #
# Title: Effect of Free Water Molecule Content on the Structure of           #
#        Mg-ATP-Dipyridylamine. Overview on Metal-Adenosine Triphosphate     #
#        Structures in Model Compounds and in Enzymes                        #
#                                                                            #
# Authors: G. Tamasi, F. Berrettini, M.B. Hursthouse, R. Cini                #
#                                                                            #
# Institutions: Department of Chemistry, University of Siena,                #
#               Via Aldo Moro 2, I-53100 Siena, Italy.                       #
#               Center for the Analysis and the Structural Determination, CIADS#
#               University of Siena, Via Aldo Moro 2, I-53100 Siena, Italy.  #
#               School of chemistry, University of Southampton,              #
#               Southampton, SO17 1BJ, United Kingdom                        #
#                                                                            #
# Email: cini@unisi.it (corresponding author)                                #
#                                                                            #
# The structures enclosed are three: mgatpDS2, mgatpDS3, caatpDS5            #
#                                                                            #
##############################################################################

######################
data_mgatpDS2
######################

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 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2sigma(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-
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P2 P 0.5765(3) 0.02408(10) 0.34836(6) 0.0375(5) Uani 1 1 d . . .
P3 P 0.4172(3) 0.12489(10) 0.32366(7) 0.0431(6) Uani 1 1 d . . .
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O5 O 0.6736(7) 0.0180(3) 0.38399(17) 0.0539(18) Uani 1 1 d . . .
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O7 O 0.4916(8) 0.0803(2) 0.35728(17) 0.0503(17) Uani 1 1 d . . .
O8 O 0.2889(8) 0.1390(3) 0.34663(19) 0.061(2) Uani 1 1 d . . .
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O9 O 0.3948(7) 0.0916(2) 0.28235(17) 0.0467(17) Uani 1 1 d . . .
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O1' O 0.3970(7) -0.2046(3) 0.39408(18) 0.0460(16) Uani 1 1 d . . .
O2' O 0.0576(7) -0.2394(3) 0.3922(2) 0.066(2) Uani 1 1 d . . .
H2'O H 0.0647 -0.2745 0.3864 0.099 Uiso 1 1 calc R . .
O3' O 0.2505(10) -0.2979(3) 0.3414(2) 0.079(3) Uani 1 1 d . . .
H3'O H 0.2488 -0.3089 0.3666 0.118 Uiso 1 1 calc R . .
O5' O 0.3285(7) -0.1113(3) 0.33645(19) 0.0499(17) Uani 1 1 d . . .
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O3WB O -0.1198(14) 0.0203(7) 0.2743(5) 0.086(5) Uani 0.633(15) 1 d P . .
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H1 H 0.2788 -0.1475 0.5999 0.048 Uiso 0.50 1 calc PR . .
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N6 N 0.2644(8) -0.0483(3) 0.5683(2) 0.0430(19) Uani 1 1 d . . .
H6A H 0.2641 -0.0465 0.5960 0.052 Uiso 1 1 calc R . .
H6B H 0.2601 -0.0166 0.5533 0.052 Uiso 1 1 calc R . .
N7 N 0.2516(8) -0.0688(3) 0.4704(2) 0.0385(18) Uani 1 1 d . . .
N9 N 0.2594(9) -0.1601(3) 0.4449(2) 0.0401(19) Uani 1 1 d . . .
N1D N 0.5996(10) 0.0595(4) 0.4806(4) 0.065(3) Uani 0.86 1 d P . .
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N2D N 0.6094(14) -0.0010(6) 0.5322(4) 0.032(3) Uani 0.50 1 d P . .
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H2DB H 0.9186 0.0390 0.5539 0.212 Uiso 0.50 1 calc PR . .
C2 C 0.2840(10) -0.2040(4) 0.5530(3) 0.043(2) Uani 1 1 d . . .
H2 H 0.2930 -0.2362 0.5713 0.051 Uiso 1 1 calc R . .
C4 C 0.2682(10) -0.1651(3) 0.4888(2) 0.034(2) Uani 1 1 d . . .
C5 C 0.2654(8) -0.1081(3) 0.5042(2) 0.0283(17) Uani 1 1 d . . .
C6 C 0.2714(9) -0.1003(3) 0.5487(3) 0.0316(19) Uani 1 1 d . . .
C8 C 0.2470(10) -0.1023(3) 0.4369(3) 0.039(2) Uani 1 1 d . . .
H8 H 0.2359 -0.0875 0.4092 0.046 Uiso 1 1 calc R . .
C1' C 0.2725(10) -0.2084(4) 0.4136(2) 0.039(2) Uani 1 1 d . . .
H1' H 0.2672 -0.2459 0.4292 0.046 Uiso 1 1 calc R . .
C2' C 0.1716(10) -0.2090(4) 0.3783(3) 0.045(2) Uani 1 1 d . . .
H2' H 0.1479 -0.1683 0.3713 0.054 Uiso 1 1 calc R . .
C3' C 0.2459(12) -0.2355(4) 0.3399(3) 0.051(3) Uani 1 1 d . . .
H3' H 0.2108 -0.2214 0.3124 0.061 Uiso 1 1 calc R . .
C4' C 0.3857(11) -0.2128(4) 0.3476(3) 0.049(3) Uani 1 1 d . . .
H4' H 0.4475 -0.2435 0.3387 0.059 Uiso 1 1 calc R . .
C5' C 0.4221(11) -0.1565(4) 0.3251(3) 0.055(3) Uani 1 1 d . . .
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H5'2 H 0.4218 -0.1625 0.2941 0.066 Uiso 1 1 calc R . .
C1D C 0.5986(11) 0.0529(4) 0.5258(4) 0.072(3) Uani 1.17 1 d P . .
C2D C 0.5883(11) 0.1030(4) 0.5489(3) 0.058(3) Uani 1 1 d . . .
H2D H 0.5797 0.1004 0.5787 0.070 Uiso 1 1 calc R . .
C3D C 0.5901(10) 0.1579(4) 0.5299(3) 0.048(2) Uani 1 1 d . . .
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C2D1 C 0.9390(17) 0.1255(9) 0.5102(8) 0.137(8) Uani 1 1 d D . .
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C5D1 C 0.9362(14) 0.0767(11) 0.4302(8) 0.151(9) Uani 1 1 d D . .
H5D1 H 0.9338 0.0604 0.4027 0.181 Uiso 1 1 calc R . .
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O2WD O 0.0000 -0.2559(5) 0.2500 0.160(10) Uani 1 2 d S . .
O3WD O 0.0038(18) -0.0628(9) 0.3251(7) 0.246(9) Uani 1 1 d . . .
O4WD O 0.2658(14) -0.1158(5) 0.2188(4) 0.141(4) Uani 1 1 d . . .
O5WD O 0.3029(17) -0.2360(6) 0.2152(5) 0.167(6) Uani 1 1 d . . .
O6WD O -0.1884(16) -0.1907(7) 0.3693(4) 0.183(6) Uani 1 1 d . . .
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P2 0.0447(13) 0.0437(12) 0.0242(9) 0.0013(9) 0.0044(10) -0.0041(13)
P3 0.0628(17) 0.0365(11) 0.0299(10) -0.0046(9) 0.0083(13) 0.0006(13)
O2 0.073(5) 0.049(4) 0.052(3) -0.001(3) 0.028(4) 0.003(4)
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O7 0.075(5) 0.041(3) 0.035(3) -0.005(3) 0.000(4) 0.007(4)
O8 0.063(5) 0.082(5) 0.038(3) -0.023(3) 0.000(4) 0.016(4)
O9 0.070(5) 0.046(3) 0.024(3) -0.009(2) 0.006(3) 0.019(4)
O10 0.120(7) 0.045(4) 0.060(4) -0.003(3) 0.008(5) -0.016(5)
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O2' 0.051(5) 0.069(5) 0.079(5) 0.002(4) 0.008(4) -0.035(4)
O3' 0.146(9) 0.036(4) 0.054(4) -0.013(3) 0.014(5) -0.020(5)
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N3 0.047(5) 0.038(4) 0.036(4) 0.005(3) -0.002(4) 0.000(4)
N6 0.048(5) 0.053(5) 0.027(3) 0.005(3) 0.002(4) 0.003(4)
N7 0.050(5) 0.034(4) 0.031(3) -0.001(3) 0.015(4) 0.001(4)
N9 0.058(6) 0.036(4) 0.027(3) -0.003(3) 0.001(4) -0.009(4)
N1D 0.035(6) 0.053(6) 0.106(9) -0.045(6) 0.009(6) -0.005(5)
N2D 0.033(8) 0.043(8) 0.021(6) 0.009(5) 0.009(6) 0.007(7)
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C4 0.042(6) 0.034(4) 0.027(4) -0.001(3) 0.000(4) -0.007(4)
C5 0.024(4) 0.034(4) 0.027(4) -0.003(3) 0.006(4) 0.004(4)
C6 0.025(5) 0.030(4) 0.040(4) -0.002(4) 0.000(4) -0.003(4)
C8 0.059(7) 0.029(4) 0.028(4) 0.001(3) 0.002(4) 0.001(5)
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C2' 0.057(6) 0.044(5) 0.034(4) 0.000(4) -0.007(5) -0.022(5)
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C5' 0.071(7) 0.043(5) 0.051(5) 0.001(4) 0.030(6) -0.013(6)
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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
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 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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Mg1 P2 3.148(2) . ?
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 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
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O7 O 0.4828(4) 0.08091(17) 0.35746(12) 0.0424(10) Uani 1 1 d . . .
O8 O 0.2796(4) 0.14157(19) 0.34601(13) 0.0459(11) Uani 1 1 d . . .
H8P H 0.2396 0.1107 0.3511 0.069 Uiso 0.50 1 calc PR . .
O9 O 0.3892(4) 0.09521(16) 0.28143(11) 0.0344(10) Uani 1 1 d . . .
O10 O 0.5032(4) 0.17948(18) 0.32214(14) 0.0509(11) Uani 1 1 d . . .
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O3' O 0.2644(4) -0.30257(16) 0.34000(13) 0.0491(11) Uani 1 1 d . . .
H3'O H 0.1904 -0.3165 0.3357 0.074 Uiso 1 1 calc R . .
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O2WA O -0.1536(4) 0.1299(2) 0.26405(14) 0.0579(12) Uani 1 1 d . . .
O3WA O -0.1279(4) 0.0004(2) 0.27076(16) 0.0672(15) Uani 1 1 d . . .
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N9 N 0.2626(5) -0.16310(19) 0.44352(15) 0.0361(12) Uani 1 1 d . . .
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C2 C 0.2921(6) -0.2061(3) 0.5532(2) 0.0433(16) Uani 1 1 d . . .
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C4 0.042(4) 0.028(3) 0.031(4) -0.005(3) 0.003(3) -0.005(3)
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C2' 0.057(4) 0.035(3) 0.025(3) -0.007(3) 0.000(3) 0.001(3)
C3' 0.071(5) 0.027(3) 0.024(3) 0.000(3) 0.002(3) -0.005(3)
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C2D 0.055(5) 0.054(4) 0.064(5) 0.006(4) 0.001(4) 0.000(4)
C3D 0.046(4) 0.038(4) 0.061(5) -0.006(3) 0.009(4) -0.009(3)
C4D 0.042(4) 0.052(4) 0.074(5) -0.006(4) 0.010(4) -0.017(3)
C5D 0.056(5) 0.054(5) 0.071(6) -0.017(4) -0.005(4) -0.011(4)
C1D1 0.048(5) 0.112(8) 0.092(7) 0.014(6) 0.011(4) 0.011(4)
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C3D1 0.051(6) 0.072(7) 0.183(13) -0.015(9) -0.013(7) 0.024(5)
C4D1 0.077(7) 0.068(7) 0.162(12) 0.030(7) 0.008(7) 0.019(5)
C5D1 0.050(5) 0.104(8) 0.119(8) 0.042(7) 0.007(5) 0.011(5)
O1WD 0.305(16) 0.071(6) 0.071(6) 0.000 0.001(9) 0.000
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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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C1D1 N1D1 C5D1 120.9(10) . . ?
N1D1 N2D1 C1D1 137.8(12) 4_556 . ?
N3 C2 N1 126.4(5) . . ?
N3 C4 N9 126.5(5) . . ?
N3 C4 C5 127.2(5) . . ?
N9 C4 C5 106.2(5) . . ?
C4 C5 N7 110.3(5) . . ?
C4 C5 C6 117.4(5) . . ?
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N6 C6 C5 123.5(5) . . ?
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N7 C8 N9 113.8(5) . . ?
O1' C1' N9 108.9(4) . . ?
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N9 C1' C2' 114.6(5) . . ?
O2' C2' C1' 109.6(5) . . ?
O2' C2' C3' 117.5(5) . . ?
C1' C2' C3' 101.1(5) . . ?
O3' C3' C4' 108.1(5) . . ?
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C4' C3' C2' 103.4(5) . . ?
O1' C4' C3' 106.3(4) . . ?
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O1' C4' C5' 109.2(5) . . ?
C3' C4' C5' 115.4(5) . . ?
O5' C5' C4' 107.9(5) . . ?
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C2D C3D C4D 118.6(7) . . ?
C5D C4D C3D 122.0(7) . . ?
N1D C5D C4D 118.3(8) . . ?
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 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
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 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2sigma(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.
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P2 P 1.0848(4) 0.51903(12) 0.85212(7) 0.0832(10) Uani 1 1 d . . .
P3 P 0.9261(4) 0.62102(12) 0.82757(8) 0.0883(11) Uani 1 1 d . . .
O2 O 0.7438(13) 0.4799(4) 0.8495(3) 0.124(3) Uani 1 1 d . . .
O3 O 0.8773(14) 0.4530(4) 0.7868(2) 0.141(5) Uani 1 1 d . . .
O4 O 0.9831(11) 0.4660(3) 0.85703(19) 0.102(3) Uani 1 1 d . . .
O5 O 1.1802(9) 0.5150(4) 0.8867(2) 0.101(3) Uani 1 1 d . . .
O6 O 1.1372(9) 0.5196(3) 0.80902(18) 0.085(2) Uani 1 1 d . . .
O7 O 0.9985(8) 0.5746(2) 0.85966(16) 0.0675(18) Uani 1 1 d . . .
O8 O 0.8017(11) 0.6397(4) 0.8497(2) 0.112(3) Uani 1 1 d . . .
H8P H 0.7644 0.6110 0.8595 0.169 Uiso 1 1 calc R . .
O9 O 0.8930(10) 0.5880(3) 0.78879(19) 0.096(3) Uani 1 1 d . . .
O10 O 1.0233(15) 0.6696(3) 0.8221(2) 0.144(5) Uani 1 1 d . . .
O1' O 0.9083(8) 0.2935(3) 0.9011(2) 0.083(2) Uani 1 1 d . . .
O2' O 0.5588(9) 0.2613(3) 0.9025(3) 0.103(3) Uani 1 1 d . . .
H2' H 0.4949 0.2679 0.8873 0.155 Uiso 1 1 calc R . .
O3' O 0.7548(14) 0.1995(3) 0.8555(2) 0.140(4) Uani 1 1 d . . .
H3' H 0.6785 0.1869 0.8580 0.210 Uiso 1 1 calc R . .
O5' O 0.8361(13) 0.3817(4) 0.8457(3) 0.135(4) Uani 1 1 d . . .
O1WA O 0.551(4) 0.6126(16) 0.8196(11) 0.178(17) Uiso 0.43(3) 1 d P . .
O1WB O 0.6119(14) 0.5653(6) 0.8081(4) 0.088(7) Uiso 0.57(3) 1 d P . .
O2WA O 0.272(2) 0.660(2) 0.7663(6) 0.103(13) Uiso 0.51(10) 1 d P . .
O2WB O 0.283(3) 0.632(3) 0.7670(8) 0.139(13) Uiso 0.49(10) 1 d P . .
O3WA O 0.375(3) 0.5269(11) 0.7698(14) 0.215(12) Uiso 0.75(7) 1 d P . .
O3WB O 0.416(5) 0.5246(19) 0.793(2) 0.12(3) Uiso 0.25(7) 1 d P . .
N1 N 0.7871(8) 0.3538(3) 1.0716(2) 0.0510(18) Uani 1 1 d . . .
H1 H 0.7930 0.3571 1.0981 0.061 Uiso 0.50 1 calc PR . .
N3 N 0.7815(7) 0.2875(3) 1.0144(2) 0.0504(18) Uani 1 1 d . . .
N6 N 0.7753(7) 0.4544(3) 1.0660(2) 0.0481(17) Uani 1 1 d . . .
H6A H 0.7794 0.4573 1.0926 0.058 Uiso 1 1 calc R . .
H6B H 0.7695 0.4854 1.0511 0.058 Uiso 1 1 calc R . .
N7 N 0.7649(6) 0.4306(3) 0.9724(2) 0.0441(16) Uani 1 1 d . . .
N9 N 0.7692(7) 0.3389(3) 0.94898(19) 0.0439(16) Uani 1 1 d . . .
N1D N 1.1121(8) 0.5588(4) 0.9800(3) 0.061(3) Uani 0.86 1 d P . .
H1D H 1.1159 0.5274 0.9654 0.073 Uiso 0.50 1 calc PR . .
N2D N 1.1176(12) 0.4994(6) 1.0328(4) 0.044(3) Uani 0.50 1 d P . .
H2DA H 1.1331 0.4982 1.0590 0.053 Uiso 0.50 1 calc PR . .
N1D1 N 0.9436(15) 0.9536(10) 1.0338(8) 0.136(7) Uani 0.86 1 d PD . .
H1D1 H 0.9392 0.9903 1.0391 0.163 Uiso 0.50 1 calc PR . .
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N2D1 N 0.9428(16) 0.9794(14) 0.9673(9) 0.125(9) Uani 0.50 1 d PD . .
H2DB H 0.9390 0.9650 0.9427 0.150 Uiso 0.50 1 calc PR . .
C2 C 0.7874(11) 0.2994(4) 1.0540(3) 0.066(3) Uani 1 1 d . . .
H2 H 0.7921 0.2677 1.0720 0.079 Uiso 1 1 calc R . .
C4 C 0.7755(8) 0.3359(3) 0.9910(2) 0.0435(19) Uani 1 1 d . . .
C5 C 0.7722(8) 0.3929(3) 1.0056(2) 0.0421(18) Uani 1 1 d . . .
C6 C 0.7780(7) 0.4021(3) 1.0481(2) 0.0373(18) Uani 1 1 d . . .
C8 C 0.7633(8) 0.3963(3) 0.9402(3) 0.045(2) Uani 1 1 d . . .
H8 H 0.7584 0.4104 0.9132 0.054 Uiso 1 1 calc R . .
C1' C 0.7783(12) 0.2908(4) 0.9209(3) 0.062(3) Uani 1 1 d . . .
H1' H 0.7719 0.2543 0.9366 0.075 Uiso 1 1 calc R . .
C2' C 0.6720(13) 0.2908(4) 0.8875(3) 0.078(3) Uani 1 1 d . . .
H2'1 H 0.6483 0.3311 0.8802 0.093 Uiso 1 1 calc R . .
C3' C 0.751(2) 0.2615(5) 0.8510(3) 0.131(7) Uani 1 1 d . . .
H3'1 H 0.7153 0.2732 0.8240 0.158 Uiso 1 1 calc R . .
C4' C 0.895(2) 0.2822(6) 0.8572(4) 0.121(6) Uani 1 1 d . . .
H4' H 0.9561 0.2509 0.8492 0.145 Uiso 1 1 calc R . .
C5' C 0.934(2) 0.3383(6) 0.8347(4) 0.145(8) Uani 1 1 d . . .
H5'1 H 1.0223 0.3507 0.8432 0.174 Uiso 1 1 calc R . .
H5'2 H 0.9339 0.3320 0.8050 0.174 Uiso 1 1 calc R . .
C1D C 1.1100(8) 0.5545(4) 1.0234(4) 0.074(3) Uani 1.17 1 d P . .
C2D C 1.1018(8) 0.6040(3) 1.0451(3) 0.052(2) Uani 1 1 d . . .
H2D H 1.0972 0.6020 1.0739 0.062 Uiso 1 1 calc R . .
C3D C 1.1000(9) 0.6572(4) 1.0264(3) 0.056(2) Uani 1 1 d . . .
H3D H 1.0970 0.6909 1.0424 0.067 Uiso 1 1 calc R . .
C4D C 1.1026(9) 0.6612(4) 0.9841(3) 0.056(2) Uani 1 1 d . . .
H4D H 1.1005 0.6974 0.9711 0.068 Uiso 1 1 calc R . .
C5D C 1.1083(8) 0.6102(4) 0.9613(3) 0.056(2) Uani 1 1 d . . .
H5D H 1.1095 0.6120 0.9325 0.067 Uiso 1 1 calc R . .
C1D1 C 0.9463(10) 0.9378(6) 0.9955(8) 0.125(6) Uani 1.17 1 d PD . .
C2D1 C 0.9408(12) 0.8773(8) 0.9856(6) 0.121(6) Uani 1 1 d D . .
H2D1 H 0.9314 0.8647 0.9584 0.145 Uiso 1 1 calc R . .
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H3D1 H 0.9546 0.7982 1.0113 0.140 Uiso 1 1 calc R . .
C4D1 C 0.9524(12) 0.8552(8) 1.0604(7) 0.130(6) Uani 1 1 d D . .
H4D1 H 0.9569 0.8288 1.0823 0.156 Uiso 1 1 calc R . .
C5D1 C 0.9472(15) 0.9166(9) 1.0661(8) 0.140(7) Uani 1 1 d D . .
H5D1 H 0.9464 0.9317 1.0928 0.168 Uiso 1 1 calc R . .
O1WD O 0.951(4) 0.7286(5) 0.7495(18) 0.16(2) Uani 0.50 1 d P . .
O2WD O 0.341(2) 0.3203(8) 0.8796(6) 0.115(6) Uani 0.50 1 d P . .
O3WD O 1.411(3) 0.4450(7) 0.8926(6) 0.148(9) Uani 0.50 1 d P . .
O4WD O 0.811(3) 0.2730(12) 0.7380(10) 0.187(11) Uiso 0.50 1 d P . .
O5WD O 0.624(5) 0.411(2) 0.7487(17) 0.281(18) Uiso 0.50 1 d P . .
O6WD O 0.328(2) 0.2804(11) 0.8610(8) 0.131(7) Uiso 0.50 1 d P . .
O7WD O 0.756(3) 0.3839(12) 0.7284(9) 0.179(10) Uiso 0.50 1 d P . .
O8WD O 1.278(4) 0.4039(16) 0.8532(12) 0.215(13) Uiso 0.50 1 d P . .

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Ca2 0.119(4) 0.265(8) 0.144(5) 0.000 -0.012(4) 0.000
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P2 0.146(3) 0.0621(15) 0.0412(13) 0.0073(12) 0.0113(16) 0.0054(19)
P3 0.167(3) 0.0604(15) 0.0373(12) -0.0041(11) -0.0151(18) 0.018(2)
O2 0.200(10) 0.078(5) 0.093(6) 0.008(5) 0.006(7) -0.049(7)
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O4 0.198(9) 0.066(4) 0.041(3) -0.009(3) 0.018(5) -0.044(5)
O5 0.140(7) 0.109(6) 0.056(4) 0.023(4) 0.009(5) 0.048(6)
O6 0.146(7) 0.071(4) 0.038(3) 0.007(3) 0.015(4) 0.010(5)
O7 0.112(5) 0.050(3) 0.041(3) -0.005(3) -0.001(4) 0.005(4)
O8 0.165(9) 0.117(6) 0.055(4) -0.020(4) -0.008(5) 0.068(6)
O9 0.162(8) 0.083(5) 0.043(4) -0.004(3) -0.016(4) 0.033(5)
O10 0.313(15) 0.057(4) 0.062(4) 0.018(3) -0.024(7) -0.062(7)
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O2' 0.130(7) 0.070(4) 0.109(6) 0.039(4) -0.057(5) -0.051(5)
O3' 0.281(14) 0.058(5) 0.081(5) -0.014(4) -0.003(7) -0.073(7)
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N2D 0.042(8) 0.058(8) 0.032(6) 0.014(6) -0.004(6) -0.002(6)
N1D1 0.056(10) 0.17(2) 0.19(2) -0.041(18) -0.002(11) 0.011(10)
N2D1 0.013(9) 0.14(2) 0.23(3) 0.04(2) -0.008(13) 0.000(12)
C2 0.085(8) 0.053(5) 0.059(6) 0.014(5) 0.007(5) 0.003(5)
C4 0.049(5) 0.041(4) 0.040(4) 0.009(4) -0.001(4) -0.008(4)
C5 0.032(4) 0.045(4) 0.050(5) 0.002(4) 0.006(4) -0.005(4)
C6 0.031(5) 0.035(4) 0.045(4) 0.002(3) 0.006(4) 0.002(4)
C8 0.047(5) 0.045(4) 0.043(4) 0.003(4) -0.007(4) -0.010(4)
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C5' 0.26(2) 0.095(9) 0.079(8) -0.049(7) 0.087(11) -0.073(12)
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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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