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_cell_volume 2037.3(15)

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_cell_measurement_temperature 298(2)

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_exptl_crystal_colour 'pale brown'

_exptl_crystal_size_max 0.24

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_exptl_crystal_density_diffrn 1.283

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_exptl_crystal_F_000 832

_exptl_absorpt_coefficient_mu 0.158

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_exptl_absorpt_process_details 'SADABS, Sheldrick(1996)'

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_diffrn_ambient_temperature 298(2)

_diffrn_radiation_wavelength 0.71073

_diffrn_radiation_typeMoK\a

_diffrn_radiation_source 'fine-focus sealed tube'

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_diffrn_measurement_device_type 'CCD area detector'

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Refinement of F^2^ against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2^, conventional R-factors R are based 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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O1 O 0.10304(8) 0.4806(3) -0.01175(7) 0.0476(4) Uani 1 1 d . . .

O2 O 0.17001(8) 0.3970(2) -0.11500(7) 0.0467(4) Uani 1 1 d . . .

O3 O 0.17791(11) 0.1361(3) -0.01991(10) 0.0697(5) Uani 1 1 d . . .

N N 0.32636(11) 0.3865(3) 0.21219(9) 0.0474(5) Uani 1 1 d . . .

C1 C 0.07430(13) 0.6796(4) -0.04283(12) 0.0511(6) Uani 1 1 d . . .

H1A H 0.1152 0.7892 -0.0313 0.061 Uiso 1 1 calcR . .

H1B H 0.0239 0.7221 -0.0249 0.061 Uiso 1 1 calcR . .

C2 C 0.05840(12) 0.6620(4) -0.11879(12) 0.0481(6) Uani 1 1 d . . .

C3 C 0.13832(14) 0.5945(4) -0.14476(12) 0.0545(6) Uani 1 1 d . . .

H3A H 0.1293 0.5781 -0.1934 0.065 Uiso 1 1 calcR . .

H3B H 0.1790 0.7056 -0.1349 0.065 Uiso 1 1 calcR . .

C4 C -0.01027(14) 0.5042(4) -0.13927(13) 0.0609(7) Uani 1 1 d . . .

H4A H -0.0178 0.4920 -0.1875 0.091 Uiso 1 1 calcR . .

H4B H -0.0604 0.5532 -0.1234 0.091 Uiso 1 1 calcR . .

H4C H 0.0041 0.3678 -0.1198 0.091 Uiso 1 1 calcR . .

C5 C 0.03728(18) 0.8836(4) -0.14601(17) 0.0814(9) Uani 1 1 d . . .

H5A H 0.0827 0.9777 -0.1337 0.122 Uiso 1 1 calcR . .

H5B H -0.0107 0.9351 -0.1273 0.122 Uiso 1 1 calcR . .

H5C H 0.0265 0.8779 -0.1943 0.122 Uiso 1 1 calcR . .

C6 C 0.26981(11) 0.4919(3) -0.00212(10) 0.0366(5) Uani 1 1 d . . .

C11 C 0.29278(11) 0.4652(3) 0.07253(10) 0.0358(5) Uani 1 1 d . . .

C12 C 0.26408(11) 0.6044(3) 0.11952(10) 0.0378(5) Uani 1 1 d . . .

C13 C 0.22040(12) 0.7943(4) 0.10111(12) 0.0455(5) Uani 1 1 d . . .

H13 H 0.2099 0.8311 0.0558 0.055 Uiso 1 1 calcR . .

C14 C 0.19399(13) 0.9222(4) 0.14882(13) 0.0551(6) Uani 1 1 d . . .

H14 H 0.1659 1.0469 0.1361 0.066 Uiso 1 1 calcR . .

C15 C 0.20847(15) 0.8687(4) 0.21749(14) 0.0620(7) Uani 1 1 d . . .

H15 H 0.1882 0.9558 0.2496 0.074 Uiso 1 1 calcR . .

C16 C 0.25127(15) 0.6933(4) 0.23727(12) 0.0568(6) Uani 1 1 d . . .

H16 H 0.2609 0.6614 0.2830 0.068 Uiso 1 1 calcR . .

C17 C 0.28194(12) 0.5560(4) 0.18934(11) 0.0433(5) Uani 1 1 d . . .

C18 C 0.35648(12) 0.2595(3) 0.16700(11) 0.0422(5) Uani 1 1 d . . .

C19 C 0.40441(13) 0.0811(4) 0.19088(12) 0.0524(6) Uani 1 1 d . . .

H19 H 0.4150 0.0591 0.2371 0.063 Uiso 1 1 calcR . .

C20 C 0.43465(13) -0.0559(4) 0.14854(13) 0.0556(6) Uani 1 1 d . . .

H20 H 0.4655 -0.1720 0.1655 0.067 Uiso 1 1 calcR . .

C21 C 0.42004(13) -0.0252(4) 0.07846(13) 0.0537(6) Uani 1 1 d . . .

H21 H 0.4417 -0.1207 0.0494 0.064 Uiso 1 1 calcR . .

C22 C 0.37488(12) 0.1419(4) 0.05277(11) 0.0449(5) Uani 1 1 d . . .

H22 H 0.3657 0.1595 0.0063 0.054 Uiso 1 1 calcR . .

C23 C 0.34125(11) 0.2907(3) 0.09583(10) 0.0381(5) Uani 1 1 d . . .

C7 C 0.31608(11) 0.5839(3) -0.04310(10) 0.0387(5) Uani 1 1 d . . .

C8 C 0.35907(12) 0.6648(4) -0.08762(10) 0.0414(5) Uani 1 1 d . . .

C9 C 0.34656(15) 0.8877(4) -0.11270(13) 0.0559(6) Uani 1 1 d . . .

H9A H 0.3034 0.9535 -0.0909 0.084 Uiso 1 1 calcR . .

H9B H 0.3316 0.8860 -0.1606 0.084 Uiso 1 1 calcR . .

H9C H 0.3966 0.9668 -0.1027 0.084 Uiso 1 1 calcR . .

C10 C 0.42310(13) 0.5338(4) -0.11799(12) 0.0569(6) Uani 1 1 d . . .

H10A H 0.4229 0.3916 -0.1005 0.085 Uiso 1 1 calcR . .

H10B H 0.4764 0.5962 -0.1066 0.085 Uiso 1 1 calcR . .

H10C H 0.4108 0.5305 -0.1662 0.085 Uiso 1 1 calcR . .

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O1 0.0458(8) 0.0663(11) 0.0311(8) 0.0059(7) 0.0065(6) -0.0106(7)

O2 0.0502(8) 0.0599(10) 0.0289(9) -0.0039(7) -0.0009(6) 0.0044(7)

O3 0.0795(11) 0.0471(10) 0.0753(13) 0.0144(9) -0.0248(9) -0.0173(8)

N 0.0507(10) 0.0645(13) 0.0268(10) 0.0031(9) 0.0031(8) -0.0016(9)

C1 0.0430(11) 0.0585(15) 0.0518(15) -0.0090(12) 0.0052(10) -0.0027(10)

C2 0.0414(10) 0.0542(14) 0.0467(14) 0.0047(11) -0.0043(9) -0.0021(9)

C3 0.0538(12) 0.0741(17) 0.0350(13) 0.0174(12) 0.0015(10) -0.0009(11)

C4 0.0516(13) 0.0745(18) 0.0536(16) -0.0042(13) -0.0076(11) -0.0089(11)

C5 0.0750(17) 0.0683(19) 0.094(2) 0.0199(17) -0.0212(16) 0.0027(14)

C6 0.0407(10) 0.0414(12) 0.0276(11) 0.0008(9) 0.0041(8) -0.0025(8)

C11 0.0361(9) 0.0455(12) 0.0257(11) 0.0015(9) 0.0037(8) -0.0092(8)

C12 0.0381(10) 0.0456(13) 0.0300(12) 0.0000(9) 0.0054(8) -0.0072(8)

C13 0.0442(11) 0.0524(14) 0.0393(13) -0.0001(10) 0.0021(9) -0.0042(9)

C14 0.0510(12) 0.0571(15) 0.0577(17) -0.0059(12) 0.0082(11) 0.0038(10)

C15 0.0620(14) 0.0782(19) 0.0490(16) -0.0190(14) 0.0207(12) -0.0012(13)

C16 0.0607(13) 0.0766(18) 0.0349(13) -0.0046(12) 0.0140(11) -0.0046(12)

C17 0.0443(10) 0.0580(14) 0.0284(12) -0.0006(10) 0.0073(9) -0.0083(10)

C18 0.0399(10) 0.0553(14) 0.0307(12) 0.0061(10) 0.0002(8) -0.0041(9)

C19 0.0486(12) 0.0724(17) 0.0349(13) 0.0130(12) -0.0015(10) 0.0031(11)

C20 0.0454(11) 0.0626(16) 0.0572(17) 0.0095(13) -0.0011(11) 0.0069(11)

C21 0.0476(12) 0.0610(16) 0.0516(16) -0.0050(12) 0.0010(11) 0.0028(10)

C22 0.0440(10) 0.0550(14) 0.0349(13) -0.0042(10) -0.0001(9) -0.0030(9)

C23 0.0365(9) 0.0475(13) 0.0298(11) 0.0022(9) 0.0009(8) -0.0067(8)

C7 0.0416(10) 0.0437(12) 0.0299(12) -0.0026(9) 0.0002(9) -0.0009(8)

C8 0.0427(10) 0.0546(14) 0.0272(11) -0.0005(10) 0.0043(9) -0.0107(9)

C9 0.0644(14) 0.0596(16) 0.0450(15) 0.0040(11) 0.0116(11) -0.0124(11)

C10 0.0514(12) 0.0725(17) 0.0482(15) -0.0019(12) 0.0121(11) -0.0034(11)

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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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P O2 1.5624(16) . ?
P O1 1.5657(16) . ?
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O1 C1 1.452(3) . ?
O2 C3 1.448(3) . ?
N C18 1.337(3) . ?
N C17 1.341(3) . ?
C1 C2 1.513(3) . ?
C1 H1A 0.9700 . ?
C1 H1B 0.9700 . ?
C2 C3 1.516(3) . ?
C2 C4 1.520(3) . ?
C2 C5 1.522(3) . ?
C3 H3A 0.9700 . ?
C3 H3B 0.9700 . ?

C4 H4A 0.9600 . ?

C4 H4B 0.9600 . ?

C4 H4C 0.9600 . ?

C5 H5A 0.9600 . ?

C5 H5B 0.9600 . ?

C5 H5C 0.9600 . ?

C6 C7 1.306(3) . ?

C6 C11 1.505(3) . ?

C11 C12 1.399(3) . ?

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C12 C17 1.424(3) . ?

C13 C14 1.351(3) . ?

C13 H13 0.9300 . ?

C14 C15 1.405(4) . ?

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C15 C16 1.343(4) . ?

C15 H15 0.9300 . ?

C16 C17 1.419(3) . ?

C16 H16 0.9300 . ?

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C18 C23 1.428(3) . ?

C19 C20 1.338(3) . ?

C19 H19 0.9300 . ?

C20 C21 1.405(3) . ?

C20 H20 0.9300 . ?

C21 C22 1.353(3) . ?

C21 H21 0.9300 . ?

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C22 H22 0.9300 . ?

C7 C8 1.294(3) . ?

C8 C9 1.495(3) . ?

C8 C10 1.508(3) . ?

C9 H9A 0.9600 . ?

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O3 P O1 112.15(10) . . ?

O2 P O1 105.45(8) . . ?

O3 P C6 112.14(10) . . ?

O2 P C6 106.95(9) . . ?

O1 P C6 107.52(9) . . ?

C1 O1 P 120.50(13) . . ?

C3 O2 P 121.49(14) . . ?

C18 N C17 118.09(18) . . ?

O1 C1 C2 112.13(18) . . ?

O1 C1 H1A 109.2 . . ?

C2 C1 H1A 109.2 . . ?

O1 C1 H1B 109.2 . . ?

C2 C1 H1B 109.2 . . ?

H1A C1 H1B 107.9 . . ?

C1 C2 C3 107.49(17) . . ?

C1 C2 C4 111.05(19) . . ?

C3 C2 C4 111.4(2) . . ?

C1 C2 C5 107.3(2) . . ?

C3 C2 C5 107.8(2) . . ?

C4 C2 C5 111.7(2) . . ?

O2 C3 C2 112.53(18) . . ?

O2 C3 H3A 109.1 . . ?

C2 C3 H3A 109.1 . . ?

O2 C3 H3B 109.1 . . ?

C2 C3 H3B 109.1 . . ?

H3A C3 H3B 107.8 . . ?

C2 C4 H4A 109.5 . . ?

C2 C4 H4B 109.5 . . ?

H4A C4 H4B 109.5 . . ?

C2 C4 H4C 109.5 . . ?

H4A C4 H4C 109.5 . . ?

H4B C4 H4C 109.5 . . ?

C2 C5 H5A 109.5 . . ?

C2 C5 H5B 109.5 . . ?

H5A C5 H5B 109.5 . . ?

C2 C5 H5C 109.5 . . ?

H5A C5 H5C 109.5 . . ?

H5B C5 H5C 109.5 . . ?

C7 C6 C11 124.64(17) . . ?

C7 C6 P 118.68(16) . . ?

C11 C6 P 116.27(13) . . ?

C12 C11 C23 119.05(18) . . ?

C12 C11 C6 121.76(18) . . ?

C23 C11 C6 119.13(18) . . ?

C11 C12 C13 123.29(19) . . ?

C11 C12 C17 118.20(19) . . ?

C13 C12 C17 118.48(19) . . ?

C14 C13 C12 120.6(2) . . ?

C14 C13 H13 119.7 . . ?

C12 C13 H13 119.7 . . ?

C13 C14 C15 120.7(2) . . ?

C13 C14 H14 119.6 . . ?

C15 C14 H14 119.6 . . ?

C16 C15 C14 120.7(2) . . ?

C16 C15 H15 119.7 . . ?

C14 C15 H15 119.7 . . ?

C15 C16 C17 120.9(2) . . ?

C15 C16 H16 119.6 . . ?

C17 C16 H16 119.6 . . ?

N C17 C16 118.2(2) . . ?

N C17 C12 123.24(19) . . ?

C16 C17 C12 118.6(2) . . ?

N C18 C19 118.4(2) . . ?

N C18 C23 123.38(19) . . ?

C19 C18 C23 118.2(2) . . ?

C20 C19 C18 121.7(2) . . ?

C20 C19 H19 119.2 . . ?

C18 C19 H19 119.2 . . ?

C19 C20 C21 120.3(2) . . ?

C19 C20 H20 119.9 . . ?

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C22 C21 C20 120.7(2) . . ?

C22 C21 H21 119.6 . . ?

C20 C21 H21 119.6 . . ?

C21 C22 C23 120.9(2) . . ?

C21 C22 H22 119.5 . . ?

C23 C22 H22 119.5 . . ?

C11 C23 C22 123.83(19) . . ?

C11 C23 C18 117.95(19) . . ?

C22 C23 C18 118.21(19) . . ?

C8 C7 C6 175.2(2) . . ?

C7 C8 C9 122.2(2) . . ?

C7 C8 C10 120.8(2) . . ?

C9 C8 C10 116.96(18) . . ?

C8 C9 H9A 109.5 . . ?

C8 C9 H9B 109.5 . . ?

H9A C9 H9B 109.5 . . ?

C8 C9 H9C 109.5 . . ?

H9A C9 H9C 109.5 . . ?

H9B C9 H9C 109.5 . . ?

C8 C10 H10A 109.5 . . ?

C8 C10 H10B 109.5 . . ?

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C8 C10 H10C 109.5 . . ?

H10A C10 H10C 109.5 . . ?

H10B C10 H10C 109.5 . . ?

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