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Stabilizing Zr and Ti Cations by Interaction With a Ferrocenyl Fragment

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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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C6 C 0.16299(13) 0.35578(11) 0.65434(8) 0.0332(3) Uani 1 1 d . . .
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C33 C -0.05979(11) 0.63213(9) 0.72777(8) 0.0262(2) Uani 1 1 d . . .
 C101 C -0.01939(11) 0.88777(9) 0.63407(8) 0.0258(2) Uani 1 1 d . . .
 C23 C 0.06105(12) 0.89515(10) 0.35898(8) 0.0313(3) Uani 1 1 d . . .
 F24 F 0.14957(11) 0.84316(8) 0.24323(6) 0.0526(3) Uani 1 1 d . . .
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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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    'x+1/2, -y+1/2, -z'
    '-x, y+1/2, -z+1/2'
    '-x+1/2, -y, z+1/2'

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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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_refine_ls_weighting_details

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_atom_sites_solution_hydrogens    geom
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'Flack H D (1983), Acta Cryst. A39, 876-881'
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F5 F 0.5073(2) 0.93722(15) 1.05046(12) 0.0334(6) Uani 1 1 d . . .
F6 F 0.5228(2) 0.75467(14) 1.02938(13) 0.0400(7) Uani 1 1 d . . .
F7 F 0.6840(2) 0.56783(17) 0.79050(19) 0.0534(9) Uani 1 1 d . . .
F8 F 0.73409(19) 0.72748(16) 0.80209(14) 0.0377(6) Uani 1 1 d . . .
F9 F 0.4745(2) 0.59300(15) 1.01642(16) 0.0478(8) Uani 1 1 d . . .
F10 F 0.7612(2) 0.73436(14) 1.03820(15) 0.0399(7) Uani 1 1 d . . .
F11 F 0.8636(2) 0.77944(19) 1.16673(15) 0.0464(7) Uani 1 1 d . . .
F12 F 0.7612(2) 1.05860(14) 1.13424(14) 0.0360(7) Uani 1 1 d . . .
F13 F 0.66566(19) 1.01743(14) 1.00001(15) 0.0337(6) Uani 1 1 d . . .
F14 F 0.5303(2) 0.84688(16) 0.77876(13) 0.0395(7) Uani 1 1 d . . .
F15 F 0.3443(3) 0.89308(18) 0.75500(15) 0.0484(8) Uani 1 1 d . . .
C1 C 0.8153(4) 0.9196(3) 1.1519(2) 0.0287(11) Uani 1 1 d . . .
C2 C 0.8126(4) 0.8380(3) 1.1263(2) 0.0282(11) Uani 1 1 d . . .
C3 C 0.7583(4) 0.8166(3) 1.0586(2) 0.0264(11) Uani 1 1 d . . .
C4 C 0.7033(3) 0.8728(3) 1.0123(2) 0.0245(10) Uani 1 1 d . . .
C5 C 0.5637(3) 0.7104(3) 0.9671(2) 0.0283(10) Uani 1 1 d . . .
C6 C 0.6284(4) 0.7515(2) 0.9157(2) 0.0230(10) Uani 1 1 d . . .
C7 C 0.6675(4) 0.6987(3) 0.8569(3) 0.0277(11) Uani 1 1 d . . .
C8 C 0.6431(4) 0.6150(3) 0.8493(3) 0.0344(12) Uani 1 1 d . . .
C9 C 0.5773(4) 0.5799(3) 0.9019(3) 0.0348(12) Uani 1 1 d . . .
C10 C 0.3322(4) 0.9420(3) 0.8887(3) 0.0346(12) Uani 1 1 d . . .
C11 C 0.3756(4) 0.9524(3) 0.9626(3) 0.0334(12) Uani 1 1 d . . .
C12 C 0.4735(4) 0.9269(3) 0.9737(2) 0.0274(11) Uani 1 1 d . . .
C13 C 0.5335(3) 0.8921(2) 0.9152(2) 0.0233(10) Uani 1 1 d . . .
C14 C 0.5374(4) 0.6273(3) 0.9627(3) 0.0323(11) Uani 1 1 d . . .
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C15 C 0.7217(4) 0.8953(3) 0.8577(3) 0.0364(13) Uani 1 1 d . . .
H15A H 0.7897 0.8742 0.8654 0.055 Uiso 1 1 calc R . .
H15B H 0.7212 0.9563 0.8643 0.055 Uiso 1 1 calc R . .
H15C H 0.6986 0.8809 0.8035 0.055 Uiso 1 1 calc R . .
C16 C 0.7624(4) 0.9779(3) 1.1088(2) 0.0263(11) Uani 1 1 d . . .
C17 C 0.7112(3) 0.9542(3) 1.0414(2) 0.0239(10) Uani 1 1 d . . .
C18 C 0.4835(4) 0.8845(2) 0.8418(2) 0.0253(11) Uani 1 1 d . . .
C19 C 0.3881(4) 0.9075(3) 0.8277(3) 0.0343(12) Uani 1 1 d . . .
C20 C 0.5821(5) 0.6842(3) 0.2269(3) 0.0426(14) Uani 1 1 d . . .
H20 H 0.6331 0.7054 0.1927 0.051 Uiso 1 1 calc R . .
C21 C 0.4798(5) 0.6836(3) 0.2100(3) 0.0407(14) Uani 1 1 d . . .
H21 H 0.4494 0.7045 0.1624 0.049 Uiso 1 1 calc R . .
C22 C 0.4307(4) 0.6478(3) 0.2739(3) 0.0329(13) Uani 1 1 d . . .
H22 H 0.3607 0.6400 0.2780 0.039 Uiso 1 1 calc R . .
C23 C 0.5017(4) 0.6244(3) 0.3325(2) 0.0345(11) Uani 1 1 d . . .
H23 H 0.4879 0.5976 0.3824 0.041 Uiso 1 1 calc R . .
C24 C 0.5961(4) 0.6475(3) 0.3042(3) 0.0404(14) Uani 1 1 d . . .
H24 H 0.6578 0.6402 0.3315 0.048 Uiso 1 1 calc R . .
C25 C 0.4556(4) 0.8792(3) 0.2133(3) 0.0392(14) Uani 1 1 d . . .
H25 H 0.4190 0.8561 0.1696 0.047 Uiso 1 1 calc R . .
C26 C 0.5588(4) 0.8821(3) 0.2204(3) 0.0367(14) Uani 1 1 d . . .
H26 H 0.6049 0.8615 0.1818 0.044 Uiso 1 1 calc R . .
C27 C 0.5838(4) 0.9199(3) 0.2933(3) 0.0379(14) Uani 1 1 d . . .
H27 H 0.6493 0.9296 0.3130 0.046 Uiso 1 1 calc R . .
C28 C 0.4942(5) 0.9411(3) 0.3324(3) 0.0373(12) Uani 1 1 d . . .
H28 H 0.4886 0.9673 0.3836 0.045 Uiso 1 1 calc R . .
C29 C 0.4151(4) 0.9170(3) 0.2831(3) 0.0364(13) Uani 1 1 d . . .
H29 H 0.3463 0.9246 0.2943 0.044 Uiso 1 1 calc R . .
C30 C 0.6005(3) 0.7133(4) 0.4879(3) 0.0344(11) Uani 1 1 d . . .
H30 H 0.6075 0.6572 0.4697 0.041 Uiso 1 1 calc R . .
C31 C 0.5884(4) 0.7366(3) 0.5688(3) 0.0341(13) Uani 1 1 d . . .
C32 C 0.5869(4) 0.6791(3) 0.6399(3) 0.0474(15) Uani 1 1 d . . .
H32A H 0.5446 0.6306 0.6279 0.071 Uiso 1 1 calc R . .
H32B H 0.5602 0.7090 0.6868 0.071 Uiso 1 1 calc R . .
H32C H 0.6548 0.6601 0.6515 0.071 Uiso 1 1 calc R . .
C33 C 0.5860(4) 0.8252(3) 0.5706(3) 0.0363(13) Uani 1 1 d . . .
H33 H 0.5792 0.8584 0.6177 0.044 Uiso 1 1 calc R . .
C34 C 0.5953(3) 0.8568(3) 0.4904(3) 0.0343(12) Uani 1 1 d . . .
H34 H 0.5975 0.9143 0.4755 0.041 Uiso 1 1 calc R . .
C35 C 0.6009(3) 0.7861(3) 0.4357(3) 0.0355(11) Uani 1 1 d . . .
C36 C 0.3502(4) 0.8545(3) 0.4753(3) 0.0340(12) Uani 1 1 d . . .
H36 H 0.3508 0.9113 0.4580 0.041 Uiso 1 1 calc R . .
C37 C 0.3516(3) 0.7820(3) 0.4247(3) 0.0322(11) Uani 1 1 d . . .
C38 C 0.3473(3) 0.7104(3) 0.4757(2) 0.0326(11) Uani 1 1 d . . .
H38 H 0.3451 0.6537 0.4580 0.039 Uiso 1 1 calc R . .
C39 C 0.3468(4) 0.7375(3) 0.5571(3) 0.0322(13) Uani 1 1 d . . .
C40 C 0.3407(4) 0.6828(3) 0.6299(3) 0.0467(15) Uani 1 1 d . . .
H40A H 0.3728 0.7110 0.6755 0.070 Uiso 1 1 calc R . .
H40B H 0.3746 0.6296 0.6191 0.070 Uiso 1 1 calc R . .
H40C H 0.2706 0.6720 0.6429 0.070 Uiso 1 1 calc R . .
C41 C 0.3477(4) 0.8260(3) 0.5554(3) 0.0339(13) Uani 1 1 d . . .
H41 H 0.3468 0.8612 0.6016 0.041 Uiso 1 1 calc R . .
B1 B 0.6479(4) 0.8528(3) 0.9245(3) 0.0248(12) Uani 1 1 d . . .
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Fe1 0.0262(3) 0.0240(3) 0.0229(3) -0.0011(3) -0.0004(3) -0.0036(3)
F1 0.046(2) 0.0465(18) 0.0352(15) -0.0058(13) -0.0098(15) -0.0027(15)

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F2 0.071(2) 0.0184(14) 0.074(2) -0.0019(14) 0.0011(18) -0.0061(15)
F3 0.039(2) 0.0507(19) 0.067(2) -0.0043(15) -0.0218(16) 0.0199(16)
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F6 0.061(2) 0.0280(13) 0.0313(12) 0.0042(10) 0.0207(14) -0.0024(13)
F7 0.070(2) 0.0324(17) 0.0578(18) -0.0142(14) 0.0176(17) 0.0049(15)
F8 0.0412(16) 0.0348(15) 0.0372(14) -0.0085(13) 0.0165(12) -0.0012(14)
F9 0.061(2) 0.0309(14) 0.0512(16) 0.0114(13) 0.0123(16) -0.0099(15)
F10 0.0586(19) 0.0211(15) 0.0401(14) -0.0018(11) -0.0141(14) 0.0132(14)
F11 0.0587(19) 0.0418(16) 0.0386(14) 0.0007(15) -0.0165(14) 0.0183(17)
F12 0.0474(19) 0.0226(14) 0.0381(14) -0.0053(11) -0.0011(14) -0.0052(13)
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F15 0.066(2) 0.0431(18) 0.0358(15) -0.0009(13) -0.0261(15) 0.0048(17)
C1 0.033(3) 0.034(3) 0.019(2) 0.001(2) 0.001(2) -0.005(2)
C2 0.033(3) 0.026(3) 0.025(2) 0.004(2) 0.002(2) 0.008(2)
C3 0.029(3) 0.022(2) 0.029(2) 0.0035(18) 0.005(2) 0.003(2)
C4 0.030(3) 0.023(2) 0.020(2) 0.0027(18) 0.006(2) 0.003(2)
C5 0.040(3) 0.021(2) 0.024(2) 0.006(2) 0.001(2) 0.004(2)
C6 0.029(3) 0.020(2) 0.020(2) 0.0033(17) 0.002(2) 0.004(2)
C7 0.028(3) 0.025(3) 0.031(2) 0.000(2) -0.001(2) 0.001(2)
C8 0.043(3) 0.027(3) 0.034(3) -0.010(2) 0.007(2) 0.010(2)
C9 0.043(4) 0.015(2) 0.046(3) -0.001(2) -0.007(3) 0.001(2)
C10 0.036(3) 0.022(3) 0.046(3) -0.001(2) -0.010(3) 0.004(2)
C11 0.038(3) 0.025(3) 0.038(3) 0.000(2) 0.008(2) 0.006(2)
C12 0.037(3) 0.026(2) 0.020(2) 0.0022(17) -0.005(2) 0.004(2)
C13 0.032(3) 0.0122(19) 0.026(2) 0.0041(17) 0.002(2) -0.005(2)
C14 0.039(3) 0.025(2) 0.033(2) 0.011(2) 0.000(2) -0.004(2)
C15 0.049(4) 0.029(3) 0.031(2) 0.005(2) 0.009(2) -0.003(2)
C16 0.027(3) 0.020(2) 0.032(2) -0.0020(19) 0.007(2) -0.003(2)
C17 0.023(3) 0.021(2) 0.028(2) 0.005(2) -0.001(2) -0.001(2)
C18 0.037(3) 0.016(2) 0.023(2) 0.0005(16) -0.002(2) 0.002(2)
C19 0.046(3) 0.023(2) 0.033(3) 0.004(2) -0.017(3) -0.001(2)
C20 0.050(4) 0.041(3) 0.036(3) -0.007(2) 0.019(3) -0.001(3)
C21 0.061(5) 0.038(3) 0.023(2) -0.0048(19) 0.000(3) -0.009(3)
C22 0.040(3) 0.033(3) 0.025(3) -0.008(2) 0.002(2) -0.016(3)
C23 0.049(3) 0.024(2) 0.030(2) -0.0063(18) -0.003(3) -0.002(3)
C24 0.043(4) 0.037(3) 0.042(3) -0.013(3) -0.002(3) 0.014(3)
C25 0.047(4) 0.041(3) 0.031(3) 0.016(2) -0.006(3) -0.005(3)
C26 0.043(4) 0.034(3) 0.033(3) 0.006(2) 0.013(3) -0.003(3)
C27 0.031(3) 0.029(3) 0.053(3) 0.015(3) -0.003(3) -0.014(3)
C28 0.056(4) 0.024(2) 0.032(2) 0.0065(18) 0.006(3) -0.001(3)
C29 0.031(3) 0.040(3) 0.039(3) 0.013(2) 0.011(3) 0.006(3)
C30 0.026(3) 0.041(3) 0.037(3) -0.006(3) -0.002(2) 0.004(3)
C31 0.026(3) 0.045(4) 0.031(2) -0.003(2) -0.003(2) -0.003(2)
C32 0.044(4) 0.057(4) 0.041(3) 0.007(3) -0.006(3) 0.011(3)
C33 0.029(3) 0.041(3) 0.039(3) -0.009(2) -0.005(2) -0.012(3)
C34 0.028(3) 0.031(3) 0.043(3) -0.007(2) 0.005(2) -0.012(2)
C35 0.031(3) 0.038(3) 0.037(2) 0.000(3) 0.012(2) 0.001(3)
C36 0.028(3) 0.034(3) 0.039(3) 0.005(2) 0.003(2) 0.001(3)
C37 0.033(3) 0.034(3) 0.030(2) 0.002(3) -0.010(2) -0.007(3)
C38 0.029(3) 0.034(3) 0.034(2) 0.001(2) -0.007(2) -0.009(3)
C39 0.025(3) 0.039(3) 0.033(3) 0.009(2) 0.001(2) -0.012(2)
C40 0.040(3) 0.060(4) 0.039(3) 0.016(2) 0.000(3) -0.017(3)
C41 0.028(3) 0.038(3) 0.035(3) -0.003(2) 0.004(2) -0.008(3)
B1 0.037(4) 0.019(3) 0.018(2) 0.002(2) 0.006(2) 0.002(3)

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_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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Zr1 C22 2.497(5) . ?
Zr1 C20 2.506(5) . ?
Zr1 C27 2.509(5) . ?
Zr1 C24 2.527(5) . ?
Zr1 C23 2.529(4) . ?
Zr1 C29 2.531(5) . ?
Zr1 C28 2.533(4) . ?
Zr1 C37 2.603(5) . ?
Zr1 H37 2.33(5) . ?
Fe1 C35 2.003(4) . ?
Fe1 C37 2.015(4) . ?
Fe1 C36 2.037(5) . ?
Fe1 C34 2.038(4) . ?
Fe1 C30 2.044(5) . ?
Fe1 C41 2.057(5) . ?
Fe1 C38 2.061(5) . ?
Fe1 C33 2.070(5) . ?
Fe1 C39 2.084(5) . ?
Fe1 C31 2.090(5) . ?
F1 C1 1.336(5) . ?
F2 C9 1.350(5) . ?
F3 C10 1.342(6) . ?
F4 C11 1.346(5) . ?
F5 C12 1.362(5) . ?
F6 C5 1.366(5) . ?
F7 C8 1.350(5) . ?
F8 C7 1.354(5) . ?
F9 C14 1.344(5) . ?
F10 C3 1.355(5) . ?
F11 C2 1.338(5) . ?
F12 C16 1.354(5) . ?
F13 C17 1.365(5) . ?
F14 C18 1.359(4) . ?
F15 C19 1.361(5) . ?
C1 C2 1.370(6) . ?
C1 C16 1.371(6) . ?
C2 C3 1.382(6) . ?
C3 C4 1.393(6) . ?
C4 C17 1.390(6) . ?
C4 B1 1.666(6) . ?
C5 C14 1.374(6) . ?
C5 C6 1.383(6) . ?
C6 C7 1.392(6) . ?
C6 B1 1.642(7) . ?
C7 C8 1.381(6) . ?
C8 C9 1.361(7) . ?
C9 C14 1.369(6) . ?
C10 C11 1.367(6) . ?
C10 C19 1.374(7) . ?
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C12 C13 1.377(6) . ?
C13 C18 1.396(6) . ?
C13 B1 1.666(7) . ?
C15 B1 1.633(7) . ?
C15 H15A 0.9800 . ?

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C15 H15B 0.9800 . ?
 C15 H15C 0.9800 . ?
 C16 C17 1.365(6) . ?
 C18 C19 1.352(6) . ?
 C20 C21 1.401(8) . ?
 C20 C24 1.423(7) . ?
 C20 H20 0.9500 . ?
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 C26 Zr1 C21 84.73(17) . . ?
 C25 Zr1 C21 78.25(16) . . ?
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 C26 Zr1 C22 115.77(16) . . ?

C25	Zr1	C22	100.93(17)	. . ?
C21	Zr1	C22	31.93(15)	. . ?
C35	Zr1	C20	106.52(19)	. . ?
C26	Zr1	C20	79.22(16)	. . ?
C25	Zr1	C20	90.76(18)	. . ?
C21	Zr1	C20	32.57(18)	. . ?
C22	Zr1	C20	53.50(18)	. . ?
C35	Zr1	C27	83.53(18)	. . ?
C26	Zr1	C27	32.44(16)	. . ?
C25	Zr1	C27	54.02(18)	. . ?
C21	Zr1	C27	116.47(17)	. . ?
C22	Zr1	C27	148.09(17)	. . ?
C20	Zr1	C27	102.74(18)	. . ?
C35	Zr1	C24	80.40(17)	. . ?
C26	Zr1	C24	107.18(18)	. . ?
C25	Zr1	C24	123.59(17)	. . ?
C21	Zr1	C24	54.12(17)	. . ?
C22	Zr1	C24	53.87(18)	. . ?
C20	Zr1	C24	32.84(16)	. . ?
C27	Zr1	C24	119.58(17)	. . ?
C35	Zr1	C23	88.93(17)	. . ?
C26	Zr1	C23	132.52(16)	. . ?
C25	Zr1	C23	131.17(16)	. . ?
C21	Zr1	C23	53.53(14)	. . ?
C22	Zr1	C23	32.63(15)	. . ?
C20	Zr1	C23	53.57(16)	. . ?
C27	Zr1	C23	151.76(18)	. . ?
C24	Zr1	C23	32.17(17)	. . ?
C35	Zr1	C29	117.95(19)	. . ?
C26	Zr1	C29	53.68(17)	. . ?
C25	Zr1	C29	32.71(16)	. . ?
C21	Zr1	C29	106.02(17)	. . ?
C22	Zr1	C29	117.69(16)	. . ?
C20	Zr1	C29	123.44(17)	. . ?
C27	Zr1	C29	53.53(16)	. . ?
C24	Zr1	C29	156.29(17)	. . ?
C23	Zr1	C29	149.43(18)	. . ?
C35	Zr1	C28	87.54(18)	. . ?
C26	Zr1	C28	53.56(16)	. . ?
C25	Zr1	C28	53.76(16)	. . ?
C21	Zr1	C28	131.86(15)	. . ?
C22	Zr1	C28	149.64(17)	. . ?
C20	Zr1	C28	132.36(16)	. . ?
C27	Zr1	C28	32.41(16)	. . ?
C24	Zr1	C28	151.25(19)	. . ?
C23	Zr1	C28	173.88(13)	. . ?
C29	Zr1	C28	31.96(16)	. . ?
C35	Zr1	C37	86.45(15)	. . ?
C26	Zr1	C37	133.61(17)	. . ?
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C22	Zr1	C37	85.42(16)	. . ?
C20	Zr1	C37	138.10(17)	. . ?
C27	Zr1	C37	118.45(17)	. . ?
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C28	Zr1	C37	86.76(17)	. . ?
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C26	Zr1	H37	122.2(13)	. . ?
C25	Zr1	H37	90.9(13)	. . ?
C21	Zr1	H37	96.4(13)	. . ?
C22	Zr1	H37	73.9(13)	. . ?
C20	Zr1	H37	126.7(13)	. . ?
C27	Zr1	H37	120.5(13)	. . ?
C24	Zr1	H37	119.9(13)	. . ?

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 H15B C15 H15C 109.5 . . ?
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Zr1	C22	H22	117.6	.	.	?
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C24	C23	H23	126.0	.	.	?
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Zr1	C23	H23	119.5	.	.	?
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Zr1	C24	H24	118.7	.	.	?
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C27	C26	H26	125.4	.	.	?
Zr1	C26	H26	117.1	.	.	?
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Fe1	C30	H30	127.8	.	.	?
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H32A	C32	H32C	109.5	.	.	?
H32B	C32	H32C	109.5	.	.	?
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 Fe1 C38 H38 127.3 . . ?
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 H40A C40 H40C 109.5 . . ?
 H40B C40 H40C 109.5 . . ?
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 Fe1 C41 H41 126.3 . . ?
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'x, y, z'
'-x, -y, -z'

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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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 F35A F 0.57069(9) 0.19205(9) -0.04587(6) 0.0424(3) Uani 1 1 d . . .
 F36B F 0.15573(8) 0.74864(7) 0.39638(5) 0.0218(2) Uani 1 1 d . . .
 F36A F 0.45842(9) 0.29260(8) 0.04307(5) 0.0341(3) Uani 1 1 d . . .
 F42B F 0.43065(10) 0.64762(9) 0.34048(6) 0.0379(3) Uani 1 1 d . . .
 F42A F 0.37033(9) 0.41586(8) -0.01079(5) 0.0314(2) Uani 1 1 d . . .
 F43B F 0.34866(11) 0.48618(9) 0.25826(5) 0.0415(3) Uani 1 1 d . . .
 F43A F 0.43368(10) 0.59183(8) 0.05479(6) 0.0353(3) Uani 1 1 d . . .
 F44B F 0.18336(12) 0.39559(8) 0.28492(6) 0.0464(3) Uani 1 1 d . . .
 F44A F 0.35748(10) 0.68668(8) 0.16687(6) 0.0378(3) Uani 1 1 d . . .
 F45B F 0.11037(10) 0.47053(8) 0.40141(6) 0.0399(3) Uani 1 1 d . . .
 F45A F 0.21423(10) 0.59952(8) 0.21229(5) 0.0356(3) Uani 1 1 d . . .
 F46B F 0.19516(8) 0.63332(7) 0.48718(5) 0.0266(2) Uani 1 1 d . . .
 F46A F 0.15521(9) 0.42202(8) 0.15098(5) 0.0310(2) Uani 1 1 d . . .
 F52B F 0.53488(9) 0.62360(8) 0.48023(5) 0.0307(2) Uani 1 1 d . . .
 F52A F 0.12882(9) 0.39196(9) -0.04402(6) 0.0387(3) Uani 1 1 d . . .
 F53B F 0.61201(9) 0.56900(8) 0.57665(6) 0.0363(3) Uani 1 1 d . . .
 F53A F -0.07708(11) 0.40383(11) -0.07767(7) 0.0512(4) Uani 1 1 d . . .
 F54B F 0.53036(9) 0.62514(8) 0.69197(6) 0.0337(3) Uani 1 1 d . . .
 F54A F -0.22552(9) 0.30202(10) -0.04759(6) 0.0423(3) Uani 1 1 d . . .
 F55B F 0.36768(10) 0.73838(9) 0.70638(5) 0.0346(3) Uani 1 1 d . . .
 F55A F -0.16172(11) 0.19179(10) 0.02137(7) 0.0489(3) Uani 1 1 d . . .
 F56B F 0.28754(9) 0.79440(8) 0.61045(5) 0.0309(2) Uani 1 1 d . . .
 F56A F 0.04264(11) 0.18186(10) 0.05881(7) 0.0482(3) Uani 1 1 d . . .
 B1B B 0.37048(15) 0.74751(13) 0.47675(9) 0.0203(4) Uani 1 1 d . . .
 B1A B 0.22818(16) 0.29381(14) 0.03654(9) 0.0217(4) Uani 1 1 d . . .
 C1A C 0.40600(15) 0.11879(13) 0.30348(10) 0.0300(4) Uani 1 1 d . . .
 H1AA H 0.4675 0.0882 0.3184 0.036 Uiso 1 1 calc R . .
 C1B C 0.3749(2) 0.37044(19) 0.80924(11) 0.0468(6) Uani 1 1 d . . .
 H1BA H 0.4106 0.4127 0.8529 0.056 Uiso 1 1 calc R . .
 C2A C 0.32889(15) 0.16341(12) 0.34163(9) 0.0269(4) Uani 1 1 d . . .
 H2AA H 0.3267 0.1699 0.3881 0.032 Uiso 1 1 calc R . .
 C2B C 0.40075(17) 0.36733(17) 0.74871(11) 0.0380(5) Uani 1 1 d . . .
 H2BA H 0.4580 0.4072 0.7421 0.046 Uiso 1 1 calc R . .
 C3A C 0.26590(16) 0.20869(12) 0.30667(10) 0.0300(4) Uani 1 1 d . . .
 H3AA H 0.2121 0.2533 0.3242 0.036 Uiso 1 1 calc R . .
 C3B C 0.34390(19) 0.29127(16) 0.70022(11) 0.0393(5) Uani 1 1 d . . .
 H3BA H 0.3544 0.2669 0.6533 0.047 Uiso 1 1 calc R . .
 C4A C 0.30267(18) 0.19057(14) 0.24597(10) 0.0360(5) Uani 1 1 d . . .
 H4AA H 0.2802 0.2212 0.2137 0.043 Uiso 1 1 calc R . .
 C4B C 0.2808(2) 0.24722(17) 0.73051(15) 0.0542(7) Uani 1 1 d . . .
 H4BA H 0.2404 0.1856 0.7090 0.065 Uiso 1 1 calc R . .
 C5A C 0.39026(17) 0.13585(15) 0.24482(11) 0.0355(5) Uani 1 1 d . . .
 H5AA H 0.4392 0.1202 0.2111 0.043 Uiso 1 1 calc R . .
 C5B C 0.3015(2) 0.2966(2) 0.79836(14) 0.0577(8) Uani 1 1 d . . .
 H5BA H 0.2769 0.2763 0.8329 0.069 Uiso 1 1 calc R . .
 C6A C 0.24922(16) -0.10805(13) 0.15109(9) 0.0299(4) Uani 1 1 d . . .
 H6AA H 0.2997 -0.1557 0.1537 0.036 Uiso 1 1 calc R . .
 C6B C 0.06154(17) 0.44325(18) 0.81813(10) 0.0389(5) Uani 1 1 d . . .
 H6BA H 0.0717 0.4864 0.8645 0.047 Uiso 1 1 calc R . .
 C7A C 0.14083(16) -0.11011(13) 0.15948(9) 0.0283(4) Uani 1 1 d . . .
 H7AA H 0.1019 -0.1594 0.1693 0.034 Uiso 1 1 calc R . .
 C7B C 0.02839(15) 0.46770(17) 0.76256(10) 0.0358(5) Uani 1 1 d . . .
 H7BA H 0.0113 0.5307 0.7633 0.043 Uiso 1 1 calc R . .

C8A C 0.09413(16) -0.03961(14) 0.14213(9) 0.0298(4) Uani 1 1 d . . .
H8AA H 0.0163 -0.0302 0.1375 0.036 Uiso 1 1 calc R . .
C8B C 0.00967(16) 0.38613(16) 0.70790(10) 0.0357(5) Uani 1 1 d . . .
H8BA H -0.0240 0.3811 0.6632 0.043 Uiso 1 1 calc R . .
C9A C 0.17315(17) 0.00830(14) 0.12407(9) 0.0317(4) Uani 1 1 d . . .
H9AA H 0.1606 0.0561 0.1035 0.038 Uiso 1 1 calc R . .
C9B C 0.03233(18) 0.31133(17) 0.72900(11) 0.0412(5) Uani 1 1 d . . .
H9BA H 0.0157 0.2446 0.7019 0.049 Uiso 1 1 calc R . .
C10A C 0.26871(17) -0.03551(15) 0.12882(9) 0.0322(4) Uani 1 1 d . . .
H10A H 0.3355 -0.0229 0.1128 0.039 Uiso 1 1 calc R . .
C10B C 0.06295(18) 0.34742(18) 0.79775(11) 0.0421(5) Uani 1 1 d . . .
H10B H 0.0729 0.3104 0.8270 0.050 Uiso 1 1 calc R . .
C11A C 0.10033(14) 0.03110(11) 0.30266(8) 0.0220(3) Uani 1 1 d . . .
C11B C 0.22897(14) 0.47626(12) 0.67973(8) 0.0218(3) Uani 1 1 d . . .
C12B C 0.31430(15) 0.47076(12) 0.64092(8) 0.0238(3) Uani 1 1 d . . .
H12A H 0.3842 0.4448 0.6481 0.029 Uiso 1 1 calc R . .
C12A C 0.08422(15) 0.10181(12) 0.36351(8) 0.0258(4) Uani 1 1 d . . .
H12B H 0.1398 0.1505 0.3924 0.031 Uiso 1 1 calc R . .
C13B C 0.28317(16) 0.50639(12) 0.59043(9) 0.0263(4) Uani 1 1 d . . .
H13A H 0.3273 0.5105 0.5570 0.032 Uiso 1 1 calc R . .
C13A C -0.02158(16) 0.09373(13) 0.37541(9) 0.0295(4) Uani 1 1 d . . .
H13B H -0.0526 0.1343 0.4139 0.035 Uiso 1 1 calc R . .
C14A C -0.07604(16) 0.01798(13) 0.32286(9) 0.0286(4) Uani 1 1 d . . .
H14A H -0.1522 -0.0045 0.3177 0.034 Uiso 1 1 calc R . .
C14B C 0.17863(16) 0.53495(12) 0.59589(9) 0.0278(4) Uani 1 1 d . . .
H14B H 0.1357 0.5625 0.5669 0.033 Uiso 1 1 calc R . .
C15B C 0.14537(15) 0.51678(12) 0.64959(8) 0.0249(4) Uani 1 1 d . . .
H15A H 0.0738 0.5287 0.6639 0.030 Uiso 1 1 calc R . .
C15A C -0.00276(15) -0.02023(12) 0.27887(9) 0.0244(3) Uani 1 1 d . . .
H15B H -0.0201 -0.0739 0.2370 0.029 Uiso 1 1 calc R . .
C16B C 0.13037(16) 0.26059(12) 0.56237(10) 0.0298(4) Uani 1 1 d . . .
H16A H 0.1253 0.2307 0.5955 0.036 Uiso 1 1 calc R . .
C16A C 0.00008(18) 0.18460(16) 0.22439(11) 0.0387(5) Uani 1 1 d . . .
H16B H 0.0618 0.1820 0.2000 0.046 Uiso 1 1 calc R . .
C17B C 0.22065(16) 0.26601(13) 0.53209(10) 0.0331(4) Uani 1 1 d . . .
H17A H 0.2902 0.2396 0.5395 0.040 Uiso 1 1 calc R . .
C17A C -0.00810(17) 0.24811(14) 0.28780(12) 0.0361(5) Uani 1 1 d . . .
H17B H 0.0464 0.2985 0.3157 0.043 Uiso 1 1 calc R . .
C18B C 0.19488(17) 0.31496(14) 0.48901(9) 0.0340(5) Uani 1 1 d . . .
H18A H 0.2430 0.3285 0.4604 0.041 Uiso 1 1 calc R . .
C18A C -0.10752(17) 0.22793(14) 0.30410(11) 0.0348(4) Uani 1 1 d . . .
H18B H -0.1358 0.2620 0.3454 0.042 Uiso 1 1 calc R . .
C19B C 0.08853(17) 0.33983(14) 0.49265(9) 0.0315(4) Uani 1 1 d . . .
H19A H 0.0485 0.3743 0.4674 0.038 Uiso 1 1 calc R . .
C19A C -0.16065(17) 0.15176(14) 0.25146(11) 0.0364(5) Uani 1 1 d . . .
H19B H -0.2330 0.1229 0.2491 0.044 Uiso 1 1 calc R . .
C20B C 0.04877(15) 0.30637(13) 0.53817(9) 0.0298(4) Uani 1 1 d . . .
H20A H -0.0239 0.3142 0.5513 0.036 Uiso 1 1 calc R . .
C20A C -0.09402(18) 0.12473(16) 0.20236(11) 0.0396(5) Uani 1 1 d . . .
H20B H -0.1107 0.0729 0.1594 0.048 Uiso 1 1 calc R . .
C21A C 0.44441(16) -0.11813(14) 0.28826(10) 0.0313(4) Uani 1 1 d . . .
H21A H 0.4630 -0.1566 0.3146 0.047 Uiso 1 1 calc R . .
H21B H 0.4989 -0.0670 0.2999 0.047 Uiso 1 1 calc R . .
H21C H 0.4404 -0.1555 0.2419 0.047 Uiso 1 1 calc R . .
C21B C 0.3052(2) 0.58568(17) 0.91790(9) 0.0431(5) Uani 1 1 d . . .
H21D H 0.3325 0.6496 0.9425 0.065 Uiso 1 1 calc R . .
H21E H 0.3573 0.5437 0.9259 0.065 Uiso 1 1 calc R . .
H21F H 0.2381 0.5733 0.9320 0.065 Uiso 1 1 calc R . .
C22A C 0.33639(16) -0.01601(13) 0.39229(9) 0.0278(4) Uani 1 1 d . . .
H22A H 0.3684 -0.0583 0.4125 0.042 Uiso 1 1 calc R . .
H22B H 0.2679 0.0006 0.4074 0.042 Uiso 1 1 calc R . .
H22C H 0.3841 0.0398 0.4045 0.042 Uiso 1 1 calc R . .
C22B C 0.4092(2) 0.60669(18) 0.81635(11) 0.0494(7) Uani 1 1 d . . .
H22D H 0.4319 0.6681 0.8486 0.074 Uiso 1 1 calc R . .
H22E H 0.4015 0.6096 0.7724 0.074 Uiso 1 1 calc R . .
H22F H 0.4625 0.5634 0.8201 0.074 Uiso 1 1 calc R . .

C23A C 0.23094(16) -0.17508(13) 0.29070(10) 0.0301(4) Uani 1 1 d . . .
 H23A H 0.2669 -0.2124 0.3139 0.045 Uiso 1 1 calc R . .
 H23B H 0.2165 -0.2112 0.2439 0.045 Uiso 1 1 calc R . .
 H23C H 0.1637 -0.1572 0.3072 0.045 Uiso 1 1 calc R . .
 C23B C 0.1986(2) 0.66025(16) 0.82803(12) 0.0546(7) Uani 1 1 d . . .
 H23D H 0.2312 0.7190 0.8600 0.082 Uiso 1 1 calc R . .
 H23E H 0.1281 0.6480 0.8382 0.082 Uiso 1 1 calc R . .
 H23F H 0.1912 0.6637 0.7842 0.082 Uiso 1 1 calc R . .
 C31B C 0.28366(13) 0.82751(11) 0.49013(8) 0.0194(3) Uani 1 1 d . . .
 C31A C 0.29253(14) 0.23676(12) -0.02448(8) 0.0216(3) Uani 1 1 d . . .
 C32B C 0.30763(15) 0.91327(12) 0.53967(8) 0.0242(3) Uani 1 1 d . . .
 C32A C 0.24773(14) 0.17639(12) -0.08589(8) 0.0234(3) Uani 1 1 d . . .
 C33B C 0.24777(16) 0.98870(12) 0.54741(9) 0.0278(4) Uani 1 1 d . . .
 C33A C 0.30561(16) 0.12336(12) -0.13272(9) 0.0273(4) Uani 1 1 d . . .
 C34B C 0.15789(15) 0.98241(12) 0.50319(9) 0.0259(4) Uani 1 1 d . . .
 C34A C 0.41440(16) 0.12817(13) -0.11963(9) 0.0282(4) Uani 1 1 d . . .
 C35B C 0.12929(14) 0.89970(12) 0.45330(8) 0.0219(3) Uani 1 1 d . . .
 C35A C 0.46402(15) 0.18652(14) -0.05986(9) 0.0282(4) Uani 1 1 d . . .
 C36B C 0.19122(13) 0.82567(11) 0.44834(8) 0.0183(3) Uani 1 1 d . . .
 C36A C 0.40317(14) 0.23775(12) -0.01467(8) 0.0245(3) Uani 1 1 d . . .
 C41B C 0.31863(13) 0.64989(11) 0.41971(8) 0.0202(3) Uani 1 1 d . . .
 C41A C 0.26603(14) 0.40557(12) 0.06919(8) 0.0218(3) Uani 1 1 d . . .
 C42B C 0.35171(15) 0.60733(13) 0.35947(9) 0.0249(4) Uani 1 1 d . . .
 C42A C 0.33356(14) 0.45572(12) 0.04682(8) 0.0235(3) Uani 1 1 d . . .
 C43B C 0.30857(17) 0.52313(13) 0.31443(9) 0.0291(4) Uani 1 1 d . . .
 C43A C 0.36626(15) 0.54800(13) 0.07897(9) 0.0261(4) Uani 1 1 d . . .
 C44B C 0.22671(17) 0.47754(12) 0.32796(9) 0.0312(4) Uani 1 1 d . . .
 C44A C 0.32794(15) 0.59643(12) 0.13560(9) 0.0273(4) Uani 1 1 d . . .
 C45B C 0.19002(15) 0.51578(12) 0.38686(9) 0.0270(4) Uani 1 1 d . . .
 C45A C 0.25645(15) 0.55225(13) 0.15851(8) 0.0259(4) Uani 1 1 d . . .
 C46B C 0.23630(14) 0.59918(12) 0.43055(8) 0.0212(3) Uani 1 1 d . . .
 C46A C 0.22769(14) 0.45944(13) 0.12558(8) 0.0234(3) Uani 1 1 d . . .
 C51B C 0.41026(13) 0.71693(12) 0.54053(8) 0.0206(3) Uani 1 1 d . . .
 C51A C 0.09876(14) 0.28946(12) 0.01193(8) 0.0234(3) Uani 1 1 d . . .
 C52B C 0.49130(14) 0.65699(12) 0.53630(8) 0.0225(3) Uani 1 1 d . . .
 C52A C 0.05967(15) 0.34290(14) -0.02407(9) 0.0267(4) Uani 1 1 d . . .
 C53B C 0.53223(14) 0.62619(12) 0.58532(9) 0.0248(3) Uani 1 1 d . . .
 C53A C -0.04647(16) 0.34955(15) -0.04302(9) 0.0319(4) Uani 1 1 d . . .
 C54B C 0.49157(14) 0.65409(12) 0.64334(9) 0.0240(3) Uani 1 1 d . . .
 C54A C -0.12173(15) 0.29867(14) -0.02776(9) 0.0314(4) Uani 1 1 d . . .
 C55B C 0.40966(14) 0.71135(12) 0.65010(8) 0.0233(3) Uani 1 1 d . . .
 C55A C -0.08867(16) 0.24337(14) 0.00685(10) 0.0325(4) Uani 1 1 d . . .
 C56B C 0.37032(14) 0.74040(12) 0.59950(8) 0.0222(3) Uani 1 1 d . . .
 C56A C 0.01901(16) 0.23975(13) 0.02584(9) 0.0287(4) Uani 1 1 d . . .
 C61B C 0.47313(15) 0.79442(14) 0.45817(10) 0.0292(4) Uani 1 1 d . . .
 H61A H 0.4994 0.8519 0.4940 0.044 Uiso 1 1 calc R . .
 H61B H 0.4515 0.8077 0.4182 0.044 Uiso 1 1 calc R . .
 H61C H 0.5298 0.7516 0.4511 0.044 Uiso 1 1 calc R . .
 C61A C 0.25691(16) 0.24771(14) 0.09270(9) 0.0291(4) Uani 1 1 d . . .
 H61D H 0.2350 0.1816 0.0744 0.044 Uiso 1 1 calc R . .
 H61E H 0.2191 0.2776 0.1297 0.044 Uiso 1 1 calc R . .
 H61F H 0.3338 0.2564 0.1076 0.044 Uiso 1 1 calc R . .
 Br1 Br 0.38888(13) 0.90320(6) 0.90121(5) 0.0976(4) Uani 0.50 1 d P . .
 C101 C 0.4839(6) 0.9793(4) 0.9778(3) 0.0556(15) Uani 0.50 1 d P . .
 C102 C 0.571(2) 0.9528(15) 0.9701(12) 0.129(8) Uani 0.50 1 d P . .
 C103 C 0.6572(6) 1.0172(8) 1.0315(6) 0.078(3) Uani 0.50 1 d P . .
 C105 C 0.5691(12) 0.9586(8) 0.9793(6) 0.047(2) Uani 0.50 1 d P . .
 C104 C 0.3545(4) 0.9270(5) 0.9311(3) 0.0362(11) Uani 0.50 1 d P . .
 C106 C 0.4776(7) 0.8983(4) 0.9157(3) 0.0509(14) Uani 0.50 1 d P . .

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F36A 0.0224(6) 0.0426(7) 0.0267(5) 0.0012(5) -0.0033(4) 0.0033(5)
F42B 0.0372(7) 0.0485(7) 0.0320(6) 0.0146(5) 0.0182(5) 0.0029(6)
F42A 0.0371(7) 0.0315(6) 0.0259(5) 0.0076(4) 0.0134(5) 0.0003(5)
F43B 0.0592(9) 0.0422(7) 0.0222(5) 0.0084(5) 0.0082(5) 0.0251(6)
F43A 0.0336(7) 0.0346(6) 0.0380(6) 0.0133(5) 0.0058(5) -0.0064(5)
F44B 0.0697(10) 0.0223(6) 0.0363(7) 0.0040(5) -0.0124(6) -0.0017(6)
F44A 0.0457(7) 0.0241(5) 0.0360(6) 0.0032(5) 0.0000(5) 0.0007(5)
F45B 0.0352(7) 0.0339(6) 0.0506(7) 0.0197(6) -0.0046(6) -0.0126(5)
F45A 0.0434(7) 0.0340(6) 0.0266(6) 0.0041(5) 0.0121(5) 0.0137(5)
F46B 0.0216(5) 0.0335(6) 0.0277(5) 0.0132(4) 0.0072(4) 0.0005(4)
F46A 0.0316(6) 0.0356(6) 0.0288(5) 0.0115(5) 0.0142(5) 0.0060(5)
F52B 0.0274(6) 0.0391(6) 0.0301(6) 0.0154(5) 0.0098(5) 0.0139(5)
F52A 0.0275(6) 0.0606(8) 0.0404(7) 0.0352(6) -0.0002(5) 0.0000(6)
F53B 0.0285(6) 0.0426(7) 0.0473(7) 0.0264(6) 0.0065(5) 0.0172(5)
F53A 0.0337(7) 0.0784(10) 0.0531(8) 0.0404(8) -0.0026(6) 0.0149(7)
F54B 0.0319(6) 0.0431(7) 0.0348(6) 0.0269(5) -0.0024(5) 0.0033(5)
F54A 0.0195(6) 0.0565(8) 0.0382(7) 0.0017(6) 0.0005(5) 0.0063(5)
F55B 0.0386(7) 0.0458(7) 0.0257(5) 0.0182(5) 0.0102(5) 0.0086(5)
F55A 0.0320(7) 0.0548(8) 0.0576(9) 0.0162(7) 0.0112(6) -0.0132(6)
F56B 0.0299(6) 0.0385(6) 0.0313(6) 0.0179(5) 0.0114(5) 0.0150(5)
F56A 0.0383(8) 0.0525(8) 0.0686(9) 0.0407(7) 0.0065(7) -0.0028(6)
B1B 0.0174(9) 0.0240(9) 0.0216(8) 0.0108(7) 0.0018(7) 0.0015(7)
B1A 0.0204(9) 0.0275(9) 0.0185(8) 0.0094(7) 0.0035(7) 0.0042(7)
C1A 0.0217(9) 0.0257(9) 0.0392(10) 0.0110(8) -0.0049(8) -0.0063(7)
C1B 0.0439(14) 0.0690(17) 0.0303(11) 0.0204(11) 0.0023(9) 0.0291(12)
C2A 0.0286(10) 0.0215(8) 0.0262(8) 0.0065(7) -0.0050(7) -0.0089(7)
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C3A 0.0306(10) 0.0164(8) 0.0387(10) 0.0078(7) -0.0035(8) -0.0051(7)
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C4A 0.0457(13) 0.0293(10) 0.0349(10) 0.0196(8) -0.0085(9) -0.0136(9)
C4B 0.0637(18) 0.0288(11) 0.0755(19) 0.0204(12) 0.0214(14) 0.0173(11)
C5A 0.0313(11) 0.0354(10) 0.0369(11) 0.0097(9) 0.0062(8) -0.0138(8)
C5B 0.0739(19) 0.0689(18) 0.0615(16) 0.0510(15) 0.0350(15) 0.0429(16)
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C6B 0.0250(10) 0.0633(15) 0.0227(9) 0.0062(9) 0.0091(8) -0.0032(9)
C7A 0.0323(10) 0.0237(8) 0.0204(8) -0.0021(7) 0.0020(7) -0.0045(7)
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C9B 0.0339(12) 0.0504(13) 0.0337(10) 0.0089(10) 0.0058(9) -0.0209(10)
C10A 0.0320(11) 0.0397(11) 0.0215(8) 0.0055(8) 0.0071(7) 0.0001(8)
C10B 0.0338(12) 0.0624(15) 0.0325(10) 0.0198(10) 0.0077(9) -0.0148(10)
C11A 0.0233(9) 0.0189(7) 0.0220(8) 0.0057(6) 0.0015(6) 0.0009(6)
C11B 0.0243(9) 0.0210(8) 0.0172(7) 0.0036(6) 0.0015(6) 0.0007(6)
C12B 0.0249(9) 0.0235(8) 0.0203(8) 0.0057(6) 0.0011(6) -0.0049(7)
C12A 0.0282(10) 0.0244(8) 0.0209(8) 0.0040(7) 0.0014(7) -0.0010(7)
C13B 0.0321(10) 0.0224(8) 0.0219(8) 0.0063(7) 0.0020(7) -0.0098(7)
C13A 0.0333(10) 0.0296(9) 0.0239(8) 0.0059(7) 0.0084(7) 0.0024(8)

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C14A 0.0266(10) 0.0281(9) 0.0319(9) 0.0104(8) 0.0081(8) -0.0005(7)
C14B 0.0395(11) 0.0202(8) 0.0225(8) 0.0079(7) -0.0001(7) 0.0009(7)
C15B 0.0299(10) 0.0218(8) 0.0212(8) 0.0053(6) 0.0031(7) 0.0054(7)
C15A 0.0249(9) 0.0200(8) 0.0252(8) 0.0045(6) 0.0037(7) -0.0009(6)
C16B 0.0346(11) 0.0182(8) 0.0311(9) 0.0034(7) 0.0013(8) -0.0052(7)
C16A 0.0382(12) 0.0446(12) 0.0465(12) 0.0292(10) 0.0136(10) 0.0160(10)
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C18B 0.0358(11) 0.0323(10) 0.0230(9) -0.0044(7) 0.0085(8) -0.0104(8)
C18A 0.0317(11) 0.0256(9) 0.0472(12) 0.0113(9) 0.0094(9) 0.0086(8)
C19B 0.0330(11) 0.0312(10) 0.0235(9) 0.0040(7) -0.0029(7) -0.0053(8)
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C20A 0.0403(12) 0.0423(12) 0.0349(11) 0.0135(9) -0.0013(9) 0.0167(10)
C21A 0.0279(10) 0.0329(10) 0.0369(10) 0.0158(8) 0.0080(8) 0.0071(8)
C21B 0.0547(15) 0.0496(13) 0.0179(9) 0.0050(9) 0.0027(9) -0.0114(11)
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C45B 0.0251(9) 0.0235(8) 0.0338(9) 0.0151(7) -0.0047(7) -0.0001(7)
C45A 0.0281(9) 0.0280(9) 0.0194(8) 0.0055(7) 0.0020(7) 0.0095(7)
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C51B 0.0161(8) 0.0231(8) 0.0235(8) 0.0105(6) -0.0004(6) -0.0004(6)
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C52B 0.0191(8) 0.0256(8) 0.0240(8) 0.0106(7) 0.0021(6) 0.0017(6)
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C61A 0.0316(10) 0.0344(10) 0.0269(9) 0.0166(8) 0.0067(8) 0.0093(8)
Br1 0.1517(12) 0.0523(5) 0.0867(7) 0.0314(5) -0.0062(7) -0.0123(6)
C101 0.078(5) 0.040(3) 0.066(4) 0.037(3) 0.019(4) 0.010(3)
C102 0.183(17) 0.115(13) 0.185(17) 0.128(13) 0.141(14) 0.097(12)
C103 0.058(4) 0.104(7) 0.122(8) 0.094(6) 0.036(5) 0.034(5)
C105 0.070(6) 0.035(4) 0.045(3) 0.021(3) 0.019(4) 0.023(4)
C104 0.023(2) 0.045(3) 0.044(3) 0.026(3) -0.009(2) -0.011(2)
C106 0.085(5) 0.033(2) 0.039(3) 0.011(2) 0.028(3) 0.005(3)

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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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Fe1B C15B 2.0465(17) . ?

Fe1B C19B 2.0502(19) . ?

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 Br1 C101 1.932(6) . ?
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C11A Zr1A C8A 88.21(6) . . ?
C4A Zr1A C8A 112.47(7) . . ?
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C8A Zr1A C7A 32.23(6) . . ?
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C4A Zr1A C6A 121.16(7) . . ?
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C10A Zr1A C6A 32.42(7) . . ?
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C8A Zr1A C6A 53.80(6) . . ?
C7A Zr1A C6A 32.62(7) . . ?
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C4A Zr1A C3A 32.78(7) . . ?
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C7A Zr1A C3A 161.04(6) . . ?
C6A Zr1A C3A 153.34(7) . . ?
C11A Zr1A C2A 89.07(6) . . ?
C4A Zr1A C2A 53.93(6) . . ?
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C7A Zr1A P1A 83.98(5) . . ?
C6A Zr1A P1A 75.81(5) . . ?
C3A Zr1A P1A 114.12(5) . . ?
C2A Zr1A P1A 82.10(4) . . ?
C1A Zr1A P1A 73.74(5) . . ?
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C11B Zr1B C9B 117.38(7) . . ?
C4B Zr1B C9B 84.32(9) . . ?
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C9B Zr1B C5B 92.76(10) . . ?
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C4B Zr1B C10B 87.54(9) . . ?
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C3B Zr1B C10B 120.22(9) . . ?
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C4B Zr1B C2B 53.85(9) . . ?
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C5B Zr1B C1B 32.15(10) . . ?
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C5B Zr1B C7B 130.05(8) . . ?
C3B Zr1B C7B 160.99(8) . . ?
C10B Zr1B C7B 53.82(8) . . ?
C8B Zr1B C7B 32.24(7) . . ?

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 C18B Fe1B C19B 40.62(8) . . ?
 C12B Fe1B C19B 152.24(8) . . ?
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 C12B Fe1B C14B 68.21(8) . . ?
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 C12B Fe1B C20B 166.25(8) . . ?
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 C15A Fe1A C19A 119.43(8) . . ?
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 C15A Fe1A C18A 151.47(8) . . ?
 C12A Fe1A C18A 120.07(8) . . ?
 C19A Fe1A C18A 40.39(8) . . ?
 C15A Fe1A C14A 40.50(7) . . ?

C12A Fe1A C14A 67.71(8) . . ?
C19A Fe1A C14A 99.61(9) . . ?
C18A Fe1A C14A 113.72(8) . . ?
C15A Fe1A C13A 67.85(7) . . ?
C12A Fe1A C13A 40.21(8) . . ?
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C18A Fe1A C13A 99.84(8) . . ?
C14A Fe1A C13A 40.30(8) . . ?
C15A Fe1A C20A 110.86(8) . . ?
C12A Fe1A C20A 167.36(9) . . ?
C19A Fe1A C20A 40.21(9) . . ?
C18A Fe1A C20A 67.59(9) . . ?
C14A Fe1A C20A 120.02(9) . . ?
C13A Fe1A C20A 152.03(9) . . ?
C15A Fe1A C17A 167.95(8) . . ?
C12A Fe1A C17A 111.10(8) . . ?
C19A Fe1A C17A 67.63(9) . . ?
C18A Fe1A C17A 40.09(8) . . ?
C14A Fe1A C17A 151.20(8) . . ?
C13A Fe1A C17A 119.61(9) . . ?
C20A Fe1A C17A 67.46(9) . . ?
C15A Fe1A C11A 41.16(7) . . ?
C12A Fe1A C11A 41.13(7) . . ?
C19A Fe1A C11A 159.23(8) . . ?
C18A Fe1A C11A 159.95(8) . . ?
C14A Fe1A C11A 69.41(7) . . ?
C13A Fe1A C11A 69.28(7) . . ?
C20A Fe1A C11A 129.45(8) . . ?
C17A Fe1A C11A 129.99(8) . . ?
C15A Fe1A C16A 131.10(8) . . ?
C12A Fe1A C16A 130.95(9) . . ?
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C18A Fe1A C16A 67.25(9) . . ?
C14A Fe1A C16A 159.43(9) . . ?
C13A Fe1A C16A 158.99(9) . . ?
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C17A Fe1A C16A 40.05(9) . . ?
C11A Fe1A C16A 117.30(8) . . ?
C23A P1A C22A 103.33(9) . . ?
C23A P1A C21A 102.72(9) . . ?
C22A P1A C21A 102.30(9) . . ?
C23A P1A Zr1A 113.16(7) . . ?
C22A P1A Zr1A 112.01(6) . . ?
C21A P1A Zr1A 121.30(7) . . ?
C22B P1B C23B 102.53(14) . . ?
C22B P1B C21B 103.22(11) . . ?
C23B P1B C21B 102.59(12) . . ?
C22B P1B Zr1B 113.76(8) . . ?
C23B P1B Zr1B 114.40(9) . . ?
C21B P1B Zr1B 118.40(8) . . ?
C61B B1B C41B 114.07(15) . . ?
C61B B1B C31B 104.58(14) . . ?
C41B B1B C31B 111.45(13) . . ?
C61B B1B C51B 109.03(14) . . ?
C41B B1B C51B 103.64(13) . . ?
C31B B1B C51B 114.33(14) . . ?
C61A B1A C51A 113.17(15) . . ?
C61A B1A C31A 105.78(14) . . ?
C51A B1A C31A 111.58(14) . . ?
C61A B1A C41A 108.20(14) . . ?
C51A B1A C41A 104.83(14) . . ?
C31A B1A C41A 113.41(14) . . ?
C5A C1A C2A 108.05(18) . . ?
C5A C1A Zr1A 73.18(11) . . ?
C2A C1A Zr1A 73.64(10) . . ?
C5B C1B C2B 108.1(2) . . ?

C5B C1B Zr1B 72.93(14) . . ?
C2B C1B Zr1B 73.85(12) . . ?
C3A C2A C1A 108.18(18) . . ?
C3A C2A Zr1A 73.43(10) . . ?
C1A C2A Zr1A 74.04(10) . . ?
C3B C2B C1B 108.4(2) . . ?
C3B C2B Zr1B 73.25(12) . . ?
C1B C2B Zr1B 73.95(13) . . ?
C2A C3A C4A 107.87(18) . . ?
C2A C3A Zr1A 74.29(10) . . ?
C4A C3A Zr1A 72.54(11) . . ?
C2B C3B C4B 108.0(2) . . ?
C2B C3B Zr1B 74.60(12) . . ?
C4B C3B Zr1B 72.47(12) . . ?
C5A C4A C3A 107.68(18) . . ?
C5A C4A Zr1A 74.60(11) . . ?
C3A C4A Zr1A 74.69(11) . . ?
C3B C4B C5B 107.4(2) . . ?
C3B C4B Zr1B 74.73(12) . . ?
C5B C4B Zr1B 74.41(13) . . ?
C1A C5A C4A 108.19(19) . . ?
C1A C5A Zr1A 74.65(11) . . ?
C4A C5A Zr1A 72.65(11) . . ?
C1B C5B C4B 108.1(2) . . ?
C1B C5B Zr1B 74.92(13) . . ?
C4B C5B Zr1B 72.68(13) . . ?
C10A C6A C7A 107.70(18) . . ?
C10A C6A Zr1A 73.39(11) . . ?
C7A C6A Zr1A 73.68(10) . . ?
C10B C6B C7B 108.38(19) . . ?
C10B C6B Zr1B 73.24(12) . . ?
C7B C6B Zr1B 73.88(11) . . ?
C8A C7A C6A 108.20(18) . . ?
C8A C7A Zr1A 73.86(10) . . ?
C6A C7A Zr1A 73.70(10) . . ?
C8B C7B C6B 107.8(2) . . ?
C8B C7B Zr1B 73.07(12) . . ?
C6B C7B Zr1B 73.52(12) . . ?
C7A C8A C9A 108.35(18) . . ?
C7A C8A Zr1A 73.91(10) . . ?
C9A C8A Zr1A 72.70(10) . . ?
C7B C8B C9B 108.09(19) . . ?
C7B C8B Zr1B 74.70(11) . . ?
C9B C8B Zr1B 72.27(12) . . ?
C8A C9A C10A 107.39(18) . . ?
C8A C9A Zr1A 74.57(11) . . ?
C10A C9A Zr1A 74.15(11) . . ?
C8B C9B C10B 107.9(2) . . ?
C8B C9B Zr1B 74.88(12) . . ?
C10B C9B Zr1B 74.72(12) . . ?
C6A C10A C9A 108.33(18) . . ?
C6A C10A Zr1A 74.19(11) . . ?
C9A C10A Zr1A 73.00(11) . . ?
C6B C10B C9B 107.8(2) . . ?
C6B C10B Zr1B 74.63(12) . . ?
C9B C10B Zr1B 72.24(12) . . ?
C12A C11A C15A 103.64(15) . . ?
C12A C11A Fe1A 68.20(10) . . ?
C15A C11A Fe1A 68.14(10) . . ?
C12A C11A Zr1A 125.39(13) . . ?
C15A C11A Zr1A 126.52(12) . . ?
Fe1A C11A Zr1A 108.77(7) . . ?
C15B C11B C12B 104.03(15) . . ?
C15B C11B Fe1B 68.19(9) . . ?
C12B C11B Fe1B 67.84(9) . . ?
C15B C11B Zr1B 125.23(13) . . ?

C12B	C11B	Zr1B	127.82(13)	. . ?
Fe1B	C11B	Zr1B	112.73(8)	. . ?
C13B	C12B	C11B	110.01(16)	. . ?
C13B	C12B	Fe1B	69.90(10)	. . ?
C11B	C12B	Fe1B	70.90(10)	. . ?
C13A	C12A	C11A	110.61(16)	. . ?
C13A	C12A	Fe1A	70.37(11)	. . ?
C11A	C12A	Fe1A	70.66(10)	. . ?
C14B	C13B	C12B	107.89(16)	. . ?
C14B	C13B	Fe1B	70.07(10)	. . ?
C12B	C13B	Fe1B	69.34(10)	. . ?
C12A	C13A	C14A	107.79(16)	. . ?
C12A	C13A	Fe1A	69.42(11)	. . ?
C14A	C13A	Fe1A	69.74(11)	. . ?
C13A	C14A	C15A	107.68(17)	. . ?
C13A	C14A	Fe1A	69.96(11)	. . ?
C15A	C14A	Fe1A	69.34(11)	. . ?
C13B	C14B	C15B	107.80(16)	. . ?
C13B	C14B	Fe1B	69.53(10)	. . ?
C15B	C14B	Fe1B	69.47(10)	. . ?
C14B	C15B	C11B	110.26(17)	. . ?
C14B	C15B	Fe1B	70.00(10)	. . ?
C11B	C15B	Fe1B	70.70(9)	. . ?
C14A	C15A	C11A	110.27(15)	. . ?
C14A	C15A	Fe1A	70.16(10)	. . ?
C11A	C15A	Fe1A	70.70(10)	. . ?
C17B	C16B	C20B	107.97(18)	. . ?
C17B	C16B	Fe1B	69.06(11)	. . ?
C20B	C16B	Fe1B	69.75(11)	. . ?
C20A	C16A	C17A	107.9(2)	. . ?
C20A	C16A	Fe1A	69.28(13)	. . ?
C17A	C16A	Fe1A	69.38(12)	. . ?
C16B	C17B	C18B	107.98(18)	. . ?
C16B	C17B	Fe1B	70.85(11)	. . ?
C18B	C17B	Fe1B	69.00(11)	. . ?
C18A	C17A	C16A	107.8(2)	. . ?
C18A	C17A	Fe1A	69.33(11)	. . ?
C16A	C17A	Fe1A	70.57(12)	. . ?
C19B	C18B	C17B	108.17(18)	. . ?
C19B	C18B	Fe1B	70.31(11)	. . ?
C17B	C18B	Fe1B	70.33(11)	. . ?
C17A	C18A	C19A	108.25(19)	. . ?
C17A	C18A	Fe1A	70.58(11)	. . ?
C19A	C18A	Fe1A	69.74(11)	. . ?
C18B	C19B	C20B	107.72(19)	. . ?
C18B	C19B	Fe1B	69.06(11)	. . ?
C20B	C19B	Fe1B	70.58(11)	. . ?
C20A	C19A	C18A	108.0(2)	. . ?
C20A	C19A	Fe1A	70.44(12)	. . ?
C18A	C19A	Fe1A	69.88(11)	. . ?
C19B	C20B	C16B	108.15(18)	. . ?
C19B	C20B	Fe1B	69.14(11)	. . ?
C16B	C20B	Fe1B	70.18(11)	. . ?
C19A	C20A	C16A	108.1(2)	. . ?
C19A	C20A	Fe1A	69.35(12)	. . ?
C16A	C20A	Fe1A	70.78(12)	. . ?
C36B	C31B	C32B	112.17(15)	. . ?
C36B	C31B	B1B	125.44(14)	. . ?
C32B	C31B	B1B	121.32(15)	. . ?
C32A	C31A	C36A	112.40(15)	. . ?
C32A	C31A	B1A	126.89(16)	. . ?
C36A	C31A	B1A	120.30(15)	. . ?
F32B	C32B	C33B	115.38(15)	. . ?
F32B	C32B	C31B	119.69(16)	. . ?
C33B	C32B	C31B	124.92(16)	. . ?
F32A	C32A	C33A	114.50(15)	. . ?

F32A	C32A	C31A	121.10(15)	.	.	?
C33A	C32A	C31A	124.39(17)	.	.	?
F33B	C33B	C34B	119.38(17)	.	.	?
F33B	C33B	C32B	120.86(17)	.	.	?
C34B	C33B	C32B	119.73(16)	.	.	?
F33A	C33A	C34A	119.79(16)	.	.	?
F33A	C33A	C32A	120.28(17)	.	.	?
C34A	C33A	C32A	119.93(17)	.	.	?
F34B	C34B	C35B	120.73(17)	.	.	?
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C34A	C35A	C36A	119.27(17)	.	.	?
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C35B	C36B	C31B	125.20(15)	.	.	?
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F36A	C36A	C31A	119.44(15)	.	.	?
C35A	C36A	C31A	125.22(17)	.	.	?
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C42B	C41B	B1B	126.70(16)	.	.	?
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F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
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C1 C 0.6022(3) 0.17288(8) 0.40377(14) 0.0443(7) Uani 1 1 d . . .
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H8B H 0.5906 0.0744 0.4375 0.118 Uiso 1 1 calc R . .
H8C H 0.7198 0.0425 0.4894 0.118 Uiso 1 1 calc R . .
C16 C 0.4417(3) 0.04128(8) 0.08746(14) 0.0395(6) Uani 1 1 d . . .
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H16C H 0.4694 0.0328 0.0364 0.059 Uiso 1 1 calc R . .
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H17B H 0.5800 -0.0503 0.2099 0.080 Uiso 1 1 calc R . .
H17C H 0.5478 -0.0470 0.1088 0.080 Uiso 1 1 calc R . .
C3 C 0.3829(3) 0.20576(9) 0.35410(15) 0.0405(6) Uani 1 1 d . . .
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F14 F 0.90419(15) 0.31990(5) 0.56387(11) 0.0554(4) Uani 1 1 d . . .
F8 F 0.88645(18) 0.06165(5) 1.00270(9) 0.0542(4) Uani 1 1 d . . .
F1 F 0.93503(14) 0.12445(5) 0.52845(8) 0.0424(3) Uani 1 1 d . . .
F7 F 1.09510(17) 0.03842(5) 0.92885(9) 0.0491(4) Uani 1 1 d . . .
C34 C 1.2059(2) 0.15837(6) 0.71566(12) 0.0230(4) Uani 1 1 d . . .
B1 B 0.9285(2) 0.16381(7) 0.70214(14) 0.0209(4) Uani 1 1 d . . .
F12 F 1.00804(18) 0.31889(5) 0.86174(12) 0.0614(5) Uani 1 1 d . . .
C29 C 1.0672(2) 0.15068(6) 0.66616(12) 0.0216(4) Uani 1 1 d . . .
C35 C 0.93872(19) 0.22145(7) 0.71115(13) 0.0237(4) Uani 1 1 d . . .

C31 C 1.1793(2) 0.12657(7) 0.55665(13) 0.0306(5) Uani 1 1 d . . .
 C46 C 1.0184(2) 0.09884(7) 0.82768(13) 0.0240(4) Uani 1 1 d . . .
 C41 C 0.9345(2) 0.13657(6) 0.79239(12) 0.0213(4) Uani 1 1 d . . .
 C36 C 0.9175(2) 0.24858(7) 0.63798(14) 0.0290(4) Uani 1 1 d . . .
 C33 C 1.3267(2) 0.15033(7) 0.69025(14) 0.0273(4) Uani 1 1 d . . .
 C43 C 0.8125(2) 0.12217(8) 0.90262(13) 0.0294(4) Uani 1 1 d . . .
 F13 F 0.96088(17) 0.36736(5) 0.71334(14) 0.0673(5) Uani 1 1 d . . .
 C28 C 0.7750(2) 0.14837(7) 0.63802(13) 0.0263(4) Uani 1 1 d . . .
 H28A H 0.7761 0.1149 0.6265 0.039 Uiso 1 1 calc R . .
 H28B H 0.7580 0.1656 0.5845 0.039 Uiso 1 1 calc R . .
 H28C H 0.6989 0.1553 0.6645 0.039 Uiso 1 1 calc R . .
 C37 C 0.9247(2) 0.29669(8) 0.63773(18) 0.0386(6) Uani 1 1 d . . .
 C30 C 1.0613(2) 0.13433(7) 0.58564(13) 0.0272(4) Uani 1 1 d . . .
 C44 C 0.9024(3) 0.08581(8) 0.93580(14) 0.0336(5) Uani 1 1 d . . .
 C32 C 1.3129(2) 0.13466(7) 0.60891(14) 0.0285(4) Uani 1 1 d . . .
 C38 C 0.9542(2) 0.32051(8) 0.7127(2) 0.0431(6) Uani 1 1 d . . .
 C42 C 0.8321(2) 0.14671(7) 0.83458(12) 0.0239(4) Uani 1 1 d . . .
 C40 C 0.9714(2) 0.24797(7) 0.78505(14) 0.0290(4) Uani 1 1 d . . .
 C45 C 1.0066(2) 0.07436(7) 0.89811(14) 0.0312(5) Uani 1 1 d . . .
 C39 C 0.9779(2) 0.29610(8) 0.78698(17) 0.0391(6) Uani 1 1 d . . .
 C11 C 0.2931(4) 0.05292(10) 0.3436(2) 0.0730(11) Uani 1 1 d . . .
 H11A H 0.2810 0.0846 0.3209 0.109 Uiso 1 1 calc R . .
 H11B H 0.3651 0.0528 0.3989 0.109 Uiso 1 1 calc R . .
 H11C H 0.2021 0.0417 0.3503 0.109 Uiso 1 1 calc R . .
 C7 C 0.7253(4) -0.01867(9) 0.36367(19) 0.0781(12) Uani 1 1 d . . .
 H7A H 0.7586 -0.0258 0.3139 0.117 Uiso 1 1 calc R . .
 H7B H 0.6468 -0.0396 0.3650 0.117 Uiso 1 1 calc R . .
 H7C H 0.8039 -0.0229 0.4155 0.117 Uiso 1 1 calc R . .
 C27 C 0.5870(2) 0.23871(7) 0.15322(14) 0.0272(4) Uani 1 1 d . . .
 H27 H 0.5963 0.2643 0.1958 0.033 Uiso 1 1 calc R . .
 H23 H 0.649(4) 0.1778(14) 0.216(3) 0.105(14) Uiso 1 1 d . . .

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 Ti1 0.0356(2) 0.01315(15) 0.01506(16) -0.00103(12) 0.00824(14) -0.00083(14)
 P1 0.0671(4) 0.0131(2) 0.0210(3) -0.0010(2) 0.0152(3) -0.0021(2)
 N1 0.0446(10) 0.0165(8) 0.0173(8) -0.0016(6) 0.0106(7) -0.0019(7)
 C22 0.0209(10) 0.0276(11) 0.0407(12) -0.0043(9) 0.0121(9) 0.0052(8)
 C23 0.0173(9) 0.0269(11) 0.0372(12) 0.0066(9) 0.0006(9) 0.0005(8)
 C21 0.0220(10) 0.0293(11) 0.0393(12) 0.0020(9) -0.0013(9) 0.0064(8)
 C25 0.0398(12) 0.0353(12) 0.0324(11) 0.0047(9) 0.0228(10) 0.0011(10)
 C4 0.0434(12) 0.0176(9) 0.0229(10) -0.0058(8) 0.0081(9) 0.0031(9)
 C14 0.0669(16) 0.0206(10) 0.0255(11) -0.0047(9) 0.0139(11) 0.0054(10)
 C24 0.0231(10) 0.0270(10) 0.0426(12) 0.0047(9) 0.0170(9) 0.0048(8)
 C18 0.0254(10) 0.0285(11) 0.0438(13) -0.0002(9) 0.0220(10) 0.0010(8)
 C5 0.0344(11) 0.0323(11) 0.0260(11) -0.0139(9) 0.0031(9) -0.0032(9)
 C20 0.0252(11) 0.0357(12) 0.0339(12) -0.0060(9) -0.0055(9) 0.0055(9)
 C15 0.0667(18) 0.0378(14) 0.0429(14) -0.0015(11) 0.0210(13) 0.0151(13)
 C19 0.0192(10) 0.0250(10) 0.0490(14) -0.0052(10) 0.0047(9) -0.0021(8)
 C26 0.0314(11) 0.0286(11) 0.0359(12) 0.0093(9) 0.0169(9) -0.0015(9)
 C1 0.0764(19) 0.0304(12) 0.0169(10) -0.0063(9) -0.0021(11) 0.0156(12)
 C13 0.078(2) 0.0480(17) 0.095(3) -0.0216(17) 0.039(2) -0.0296(16)
 C9 0.072(2) 0.0368(14) 0.0462(16) -0.0075(12) -0.0154(14) 0.0162(13)
 C6 0.105(2) 0.0238(12) 0.0238(12) 0.0018(9) 0.0004(13) 0.0134(13)
 C2 0.106(2) 0.0287(12) 0.0237(11) -0.0104(9) 0.0344(14) -0.0222(14)
 C8 0.171(4) 0.0354(15) 0.0252(13) 0.0022(11) 0.0201(18) 0.0086(19)
 C16 0.0640(16) 0.0287(12) 0.0243(11) -0.0063(9) 0.0100(11) 0.0066(11)
 C17 0.105(2) 0.0183(11) 0.0370(13) -0.0072(10) 0.0197(15) 0.0061(13)
 C3 0.0415(13) 0.0528(15) 0.0330(12) -0.0249(11) 0.0202(10) -0.0079(11)

C10 0.100(2) 0.0280(13) 0.0644(19) -0.0095(12) 0.0508(19) -0.0225(14)
 C12 0.168(4) 0.0279(14) 0.092(3) -0.0047(16) 0.080(3) -0.030(2)
 F5 0.0247(6) 0.0355(7) 0.0324(7) -0.0122(5) 0.0032(5) -0.0025(5)
 F3 0.0366(7) 0.0456(8) 0.0533(8) 0.0068(7) 0.0292(7) 0.0075(6)
 F10 0.0270(6) 0.0333(7) 0.0341(7) -0.0024(5) 0.0080(5) 0.0097(5)
 F11 0.0410(7) 0.0314(7) 0.0322(7) -0.0082(5) -0.0049(6) 0.0042(6)
 F4 0.0200(6) 0.0428(8) 0.0588(9) -0.0126(7) 0.0083(6) -0.0052(5)
 F6 0.0379(7) 0.0274(6) 0.0433(7) 0.0079(5) 0.0223(6) 0.0129(5)
 F2 0.0537(9) 0.0611(9) 0.0259(7) -0.0004(6) 0.0167(6) 0.0188(7)
 F15 0.0351(7) 0.0445(8) 0.0325(7) 0.0124(6) 0.0096(6) 0.0002(6)
 F9 0.0400(7) 0.0537(8) 0.0389(7) -0.0088(6) 0.0243(6) -0.0019(6)
 F14 0.0376(8) 0.0468(9) 0.0854(12) 0.0411(8) 0.0229(8) 0.0096(7)
 F8 0.0789(11) 0.0513(9) 0.0434(8) 0.0177(7) 0.0355(8) 0.0043(8)
 F1 0.0319(7) 0.0638(9) 0.0272(7) -0.0139(6) 0.0011(5) 0.0054(6)
 F7 0.0655(10) 0.0360(8) 0.0509(9) 0.0220(7) 0.0248(8) 0.0220(7)
 C34 0.0251(10) 0.0175(9) 0.0263(10) -0.0008(8) 0.0074(8) -0.0018(7)
 B1 0.0196(10) 0.0206(10) 0.0211(10) -0.0009(8) 0.0032(8) 0.0005(8)
 F12 0.0596(10) 0.0342(8) 0.0824(12) -0.0298(8) 0.0067(9) -0.0022(7)
 C29 0.0241(9) 0.0164(9) 0.0238(9) 0.0021(7) 0.0060(8) 0.0000(7)
 C35 0.0137(8) 0.0213(9) 0.0337(11) 0.0033(8) 0.0026(8) 0.0022(7)
 C31 0.0418(12) 0.0279(11) 0.0245(10) 0.0051(8) 0.0136(9) 0.0086(9)
 C46 0.0251(10) 0.0214(10) 0.0278(10) -0.0015(8) 0.0110(8) 0.0013(8)
 C41 0.0220(9) 0.0201(9) 0.0211(9) -0.0028(7) 0.0048(7) -0.0020(7)
 C36 0.0168(9) 0.0312(11) 0.0386(12) 0.0068(9) 0.0072(9) 0.0024(8)
 C33 0.0219(10) 0.0185(9) 0.0410(12) 0.0015(8) 0.0080(9) -0.0028(8)
 C43 0.0316(11) 0.0326(11) 0.0279(10) -0.0082(9) 0.0147(9) -0.0033(9)
 F13 0.0536(10) 0.0174(7) 0.1333(17) 0.0055(8) 0.0302(10) 0.0014(6)
 C28 0.0226(10) 0.0295(11) 0.0249(10) -0.0015(8) 0.0037(8) -0.0046(8)
 C37 0.0195(10) 0.0309(12) 0.0668(17) 0.0221(12) 0.0147(10) 0.0056(9)
 C30 0.0273(10) 0.0274(10) 0.0251(10) 0.0018(8) 0.0042(8) 0.0040(8)
 C44 0.0459(13) 0.0314(11) 0.0267(11) 0.0026(9) 0.0155(10) -0.0040(10)
 C32 0.0301(11) 0.0219(10) 0.0391(12) 0.0069(9) 0.0189(9) 0.0050(8)
 C38 0.0239(11) 0.0178(10) 0.087(2) 0.0041(12) 0.0145(12) 0.0012(9)
 C42 0.0223(9) 0.0237(10) 0.0246(10) -0.0044(8) 0.0046(8) 0.0013(8)
 C40 0.0194(9) 0.0245(10) 0.0382(12) -0.0027(9) -0.0002(9) 0.0019(8)
 C45 0.0408(12) 0.0216(10) 0.0313(11) 0.0050(8) 0.0099(9) 0.0051(9)
 C39 0.0254(11) 0.0252(11) 0.0629(16) -0.0119(11) 0.0058(11) 0.0008(9)
 C11 0.116(3) 0.0424(16) 0.090(2) -0.0145(16) 0.077(2) -0.0276(18)
 C7 0.144(3) 0.0276(14) 0.0422(16) 0.0035(12) -0.0075(19) 0.0268(17)
 C27 0.0229(10) 0.0235(10) 0.0347(11) 0.0027(9) 0.0071(8) -0.0046(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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Fe1 C23 2.002(2) . ?
 Fe1 C18 2.008(2) . ?
 Fe1 C22 2.0414(19) . ?
 Fe1 C19 2.047(2) . ?
 Fe1 C24 2.0485(19) . ?
 Fe1 C27 2.056(2) . ?
 Fe1 C25 2.069(2) . ?
 Fe1 C20 2.070(2) . ?
 Fe1 C21 2.072(2) . ?

Fe1 C26 2.075(2) . ?
 Fe1 Ti1 2.7112(4) . ?
 Ti1 N1 1.7882(16) . ?
 Ti1 C18 2.244(2) . ?
 Ti1 C23 2.337(2) . ?
 Ti1 C2 2.337(2) . ?
 Ti1 C1 2.356(2) . ?
 Ti1 C3 2.385(2) . ?
 Ti1 C5 2.409(2) . ?
 Ti1 C4 2.4311(19) . ?
 P1 N1 1.6108(16) . ?
 P1 C14 1.886(2) . ?
 P1 C6 1.890(3) . ?
 P1 C10 1.894(3) . ?
 C22 C21 1.409(3) . ?
 C22 C18 1.442(3) . ?
 C23 C24 1.430(3) . ?
 C23 C27 1.435(3) . ?
 C21 C20 1.418(3) . ?
 C25 C24 1.409(3) . ?
 C25 C26 1.421(3) . ?
 C4 C5 1.388(3) . ?
 C4 C3 1.400(3) . ?
 C14 C16 1.535(3) . ?
 C14 C15 1.542(4) . ?
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 C26 C27 1.409(3) . ?
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 C9 C6 1.542(4) . ?
 C6 C8 1.546(4) . ?
 C6 C7 1.554(3) . ?
 C2 C3 1.409(4) . ?
 C10 C11 1.539(4) . ?
 C10 C12 1.552(4) . ?
 F5 C34 1.361(2) . ?
 F3 C32 1.347(2) . ?
 F10 C42 1.357(2) . ?
 F11 C40 1.349(3) . ?
 F4 C33 1.348(2) . ?
 F6 C46 1.363(2) . ?
 F2 C31 1.350(2) . ?
 F15 C36 1.351(3) . ?
 F9 C43 1.344(2) . ?
 F14 C37 1.348(3) . ?
 F8 C44 1.343(2) . ?
 F1 C30 1.354(2) . ?
 F7 C45 1.351(2) . ?
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 B1 C41 1.661(3) . ?
 B1 C29 1.664(3) . ?
 B1 C35 1.665(3) . ?
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 C31 C32 1.365(3) . ?
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 C46 C41 1.385(3) . ?
 C41 C42 1.396(3) . ?

C36 C37 1.385(3) . ?
 C33 C32 1.378(3) . ?
 C43 C44 1.376(3) . ?
 C43 C42 1.378(3) . ?
 F13 C38 1.349(3) . ?
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 C38 C39 1.368(4) . ?
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C23 Fe1 C18 111.43(9) . . ?
 C23 Fe1 C22 127.55(9) . . ?
 C18 Fe1 C22 41.71(8) . . ?
 C23 Fe1 C19 126.81(9) . . ?
 C18 Fe1 C19 41.50(9) . . ?
 C22 Fe1 C19 68.20(8) . . ?
 C23 Fe1 C24 41.32(9) . . ?
 C18 Fe1 C24 126.92(9) . . ?
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 C19 Fe1 C24 109.55(9) . . ?
 C23 Fe1 C27 41.40(8) . . ?
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 C22 Fe1 C27 109.50(9) . . ?
 C19 Fe1 C27 164.33(9) . . ?
 C24 Fe1 C27 68.49(9) . . ?
 C23 Fe1 C25 68.65(9) . . ?
 C18 Fe1 C25 160.35(9) . . ?
 C22 Fe1 C25 153.92(9) . . ?
 C19 Fe1 C25 121.60(9) . . ?
 C24 Fe1 C25 40.03(9) . . ?
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 C23 Fe1 C20 159.41(9) . . ?
 C18 Fe1 C20 69.29(10) . . ?
 C22 Fe1 C20 67.59(9) . . ?
 C19 Fe1 C20 40.03(9) . . ?
 C24 Fe1 C20 120.71(9) . . ?
 C27 Fe1 C20 154.86(9) . . ?
 C25 Fe1 C20 103.51(10) . . ?
 C23 Fe1 C21 160.54(9) . . ?
 C18 Fe1 C21 69.36(9) . . ?
 C22 Fe1 C21 40.05(9) . . ?
 C19 Fe1 C21 67.52(9) . . ?
 C24 Fe1 C21 153.83(9) . . ?
 C27 Fe1 C21 121.44(9) . . ?
 C25 Fe1 C21 117.55(9) . . ?
 C20 Fe1 C21 40.03(9) . . ?
 C23 Fe1 C26 68.62(9) . . ?
 C18 Fe1 C26 159.44(9) . . ?
 C22 Fe1 C26 120.80(9) . . ?
 C19 Fe1 C26 155.08(9) . . ?
 C24 Fe1 C26 67.66(8) . . ?
 C27 Fe1 C26 39.91(8) . . ?
 C25 Fe1 C26 40.12(9) . . ?
 C20 Fe1 C26 118.37(9) . . ?
 C21 Fe1 C26 103.56(9) . . ?
 C23 Fe1 Ti1 57.10(7) . . ?
 C18 Fe1 Ti1 54.34(7) . . ?
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C19 Fe1 Ti1 81.46(7) . . ?
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 C21 Fe1 Ti1 120.17(7) . . ?
 C26 Fe1 Ti1 121.58(6) . . ?
 N1 Ti1 C18 103.14(8) . . ?
 N1 Ti1 C23 103.23(8) . . ?
 C18 Ti1 C23 92.63(7) . . ?
 N1 Ti1 C2 100.33(8) . . ?
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 C23 Ti1 C2 141.52(9) . . ?
 N1 Ti1 C1 100.50(8) . . ?
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 C23 Ti1 C1 110.43(9) . . ?
 C2 Ti1 C1 34.65(10) . . ?
 N1 Ti1 C3 129.79(8) . . ?
 C18 Ti1 C3 84.70(8) . . ?
 C23 Ti1 C3 126.17(8) . . ?
 C2 Ti1 C3 34.70(9) . . ?
 C1 Ti1 C3 57.30(9) . . ?
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 C18 Ti1 C5 126.33(8) . . ?
 C23 Ti1 C5 84.85(8) . . ?
 C2 Ti1 C5 56.74(9) . . ?
 C1 Ti1 C5 34.06(8) . . ?
 C3 Ti1 C5 56.30(8) . . ?
 N1 Ti1 C4 155.53(7) . . ?
 C18 Ti1 C4 93.82(8) . . ?
 C23 Ti1 C4 93.34(8) . . ?
 C2 Ti1 C4 56.57(8) . . ?
 C1 Ti1 C4 56.30(8) . . ?
 C3 Ti1 C4 33.78(8) . . ?
 C5 Ti1 C4 33.33(7) . . ?
 N1 Ti1 Fe1 109.58(5) . . ?
 C18 Ti1 Fe1 46.63(5) . . ?
 C23 Ti1 Fe1 46.00(5) . . ?
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 C1 Ti1 Fe1 144.95(7) . . ?
 C3 Ti1 Fe1 111.03(7) . . ?
 C5 Ti1 Fe1 110.92(6) . . ?
 C4 Ti1 Fe1 94.89(5) . . ?
 N1 P1 C14 108.82(9) . . ?
 N1 P1 C6 108.41(10) . . ?
 C14 P1 C6 109.66(12) . . ?
 N1 P1 C10 107.47(11) . . ?
 C14 P1 C10 110.28(12) . . ?
 C6 P1 C10 112.11(15) . . ?
 P1 N1 Ti1 168.68(11) . . ?
 C21 C22 C18 109.08(19) . . ?
 C21 C22 Fe1 71.16(12) . . ?
 C18 C22 Fe1 67.89(11) . . ?
 C24 C23 C27 107.42(19) . . ?
 C24 C23 Fe1 71.07(12) . . ?
 C27 C23 Fe1 71.28(12) . . ?
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 C27 C23 Ti1 113.44(15) . . ?
 Fe1 C23 Ti1 76.90(7) . . ?
 C22 C21 C20 108.01(19) . . ?
 C22 C21 Fe1 68.79(11) . . ?
 C20 C21 Fe1 69.90(12) . . ?
 C24 C25 C26 108.4(2) . . ?
 C24 C25 Fe1 69.21(11) . . ?
 C26 C25 Fe1 70.16(11) . . ?
 C5 C4 C3 108.4(2) . . ?

C5 C4 Ti1 72.45(11) . . ?
C3 C4 Ti1 71.31(12) . . ?
C16 C14 C15 106.1(2) . . ?
C16 C14 C17 108.9(2) . . ?
C15 C14 C17 109.3(2) . . ?
C16 C14 P1 108.75(15) . . ?
C15 C14 P1 109.56(16) . . ?
C17 C14 P1 113.93(16) . . ?
C25 C24 C23 107.95(19) . . ?
C25 C24 Fe1 70.76(12) . . ?
C23 C24 Fe1 67.61(11) . . ?
C19 C18 C22 105.55(19) . . ?
C19 C18 Fe1 70.71(12) . . ?
C22 C18 Fe1 70.40(11) . . ?
C19 C18 Ti1 115.67(14) . . ?
C22 C18 Ti1 115.59(15) . . ?
Fe1 C18 Ti1 79.03(7) . . ?
C4 C5 C1 108.5(2) . . ?
C4 C5 Ti1 74.22(12) . . ?
C1 C5 Ti1 70.89(12) . . ?
C19 C20 C21 108.1(2) . . ?
C19 C20 Fe1 69.09(12) . . ?
C21 C20 Fe1 70.07(12) . . ?
C20 C19 C18 109.13(19) . . ?
C20 C19 Fe1 70.88(12) . . ?
C18 C19 Fe1 67.79(11) . . ?
C27 C26 C25 108.35(19) . . ?
C27 C26 Fe1 69.32(11) . . ?
C25 C26 Fe1 69.72(12) . . ?
C5 C1 C2 107.7(2) . . ?
C5 C1 Ti1 75.05(12) . . ?
C2 C1 Ti1 71.96(13) . . ?
C9 C6 C8 107.4(2) . . ?
C9 C6 C7 109.0(3) . . ?
C8 C6 C7 107.6(2) . . ?
C9 C6 P1 109.75(17) . . ?
C8 C6 P1 109.3(2) . . ?
C7 C6 P1 113.59(19) . . ?
C1 C2 C3 108.2(2) . . ?
C1 C2 Ti1 73.39(13) . . ?
C3 C2 Ti1 74.51(13) . . ?
C4 C3 C2 107.2(2) . . ?
C4 C3 Ti1 74.91(12) . . ?
C2 C3 Ti1 70.79(13) . . ?
C13 C10 C11 105.9(3) . . ?
C13 C10 C12 109.4(3) . . ?
C11 C10 C12 108.7(2) . . ?
C13 C10 P1 109.68(19) . . ?
C11 C10 P1 109.56(19) . . ?
C12 C10 P1 113.4(3) . . ?
F5 C34 C33 115.90(17) . . ?
F5 C34 C29 118.96(17) . . ?
C33 C34 C29 125.14(19) . . ?
C28 B1 C41 104.01(15) . . ?
C28 B1 C29 113.67(16) . . ?
C41 B1 C29 112.28(15) . . ?
C28 B1 C35 110.44(16) . . ?
C41 B1 C35 113.86(16) . . ?
C29 B1 C35 102.90(15) . . ?
C30 C29 C34 112.57(18) . . ?
C30 C29 B1 126.36(17) . . ?
C34 C29 B1 120.96(17) . . ?
C40 C35 C36 112.59(18) . . ?
C40 C35 B1 128.08(18) . . ?
C36 C35 B1 119.30(18) . . ?
F2 C31 C32 119.21(19) . . ?

F2 C31 C30 120.8(2) . . ?
 C32 C31 C30 119.93(19) . . ?
 F6 C46 C45 114.21(17) . . ?
 F6 C46 C41 121.07(17) . . ?
 C45 C46 C41 124.70(18) . . ?
 C46 C41 C42 112.25(17) . . ?
 C46 C41 B1 127.67(17) . . ?
 C42 C41 B1 119.41(17) . . ?
 F15 C36 C37 115.6(2) . . ?
 F15 C36 C35 119.96(19) . . ?
 C37 C36 C35 124.4(2) . . ?
 F4 C33 C34 121.20(19) . . ?
 F4 C33 C32 119.64(18) . . ?
 C34 C33 C32 119.16(19) . . ?
 F9 C43 C44 119.67(19) . . ?
 F9 C43 C42 120.85(19) . . ?
 C44 C43 C42 119.47(19) . . ?
 F14 C37 C38 120.0(2) . . ?
 F14 C37 C36 120.2(2) . . ?
 C38 C37 C36 119.8(2) . . ?
 F1 C30 C31 114.43(18) . . ?
 F1 C30 C29 121.15(18) . . ?
 C31 C30 C29 124.42(19) . . ?
 F8 C44 C45 120.9(2) . . ?
 F8 C44 C43 120.6(2) . . ?
 C45 C44 C43 118.45(19) . . ?
 F3 C32 C31 120.6(2) . . ?
 F3 C32 C33 120.60(19) . . ?
 C31 C32 C33 118.76(18) . . ?
 F13 C38 C37 120.4(2) . . ?
 F13 C38 C39 120.6(3) . . ?
 C37 C38 C39 118.9(2) . . ?
 F10 C42 C43 115.28(17) . . ?
 F10 C42 C41 119.64(17) . . ?
 C43 C42 C41 125.08(19) . . ?
 F11 C40 C39 114.9(2) . . ?
 F11 C40 C35 120.68(18) . . ?
 C39 C40 C35 124.4(2) . . ?
 F7 C45 C44 119.61(19) . . ?
 F7 C45 C46 120.42(19) . . ?
 C44 C45 C46 119.95(19) . . ?
 F12 C39 C38 120.0(2) . . ?
 F12 C39 C40 120.2(2) . . ?
 C38 C39 C40 119.8(2) . . ?
 C26 C27 C23 107.80(19) . . ?
 C26 C27 Fe1 70.77(12) . . ?
 C23 C27 Fe1 67.31(11) . . ?

_diffn_measured_fraction_theta_max	0.999
_diffn_reflns_theta_full	27.47
_diffn_measured_fraction_theta_full	0.999
_refine_diff_density_max	0.350
_refine_diff_density_min	-0.300
_refine_diff_density_rms	0.052
#===end	