checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mhw01_sq

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: mhw01_sq

Bond precision: C-C = 0.0184 A Wavelength=0.71000

Cell: a=24.5588(14) b=25.8908(15) c=34.1752(18)
alpha=85.542(3) beta=84.761(4) gamma=83.319(3)
Temperature: 100 K

	Calculated	Reported
Volume	21443(2)	21443(2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C264 H144 N24 O32 P8 Pd6, 4.6(B F4), 7.8(C2 H6 O S) [+ solvent]	?
Sum formula	C279.60 H190.80 B4.60 F18.40 N24 O39.80 P8 Pd6 S7.80 [+ solvent	C280 H192 B4.60 F18.40 N24 O40 P8 Pd6 S8
Mr	6058.88	6074.53
Dx,g cm-3	0.938	0.941
Z	2	2
Mu (mm-1)	0.370	0.371
F000	6128.4	6145.0
F000'	6122.83	
h,k,lmax	24,25,34	24,25,34
Nref	44930	44832
Tmin,Tmax	0.928,0.928	0.010,0.082
Tmin'	0.928	

Correction method= # Reported T Limits: Tmin=0.010 Tmax=0.082
AbsCorr = MULTI-SCAN

Data completeness= 0.998 Theta(max)= 20.793

R(reflections)= 0.1407(20672) wR2(reflections)= 0.5240(44832)

S = 1.349 Npar= 3520

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level A

THETM01_ALERT_3_A The value of sine(theta_max)/wavelength is less than 0.550
Calculated sin(theta_max)/wavelength = 0.5000

Author Response: Despite the use of a long exposure time per degree for high resolution data on a microfocus sealed X-ray source, few reflections at greater than 1.0 A were observed and the data was trimmed accordingly.

PLAT084_ALERT_3_A High wR2 Value (i.e. > 0.25) ..... 0.52 Report

Author Response: The crystal rapidly loses solvent after removal from the mother liquor, resulting in poor crystal quality. Nevertheless geometry and ADP restraints ensure a chemically and physically meaningful structural model.

PLAT973_ALERT_2_A Check Calcd Positive Resid. Density on Pd2_1 2.27 eA-3

Author Response: The large residual hole is around the Pd atoms center, probably due to difficulties in absorption correction.

PLAT973_ALERT_2_A Check Calcd Positive Resid. Density on Pd1_1 2.13 eA-3

Author Response: The large residual hole is around the Pd atoms center, probably due to difficulties in absorption correction.

Alert level B

PLAT973_ALERT_2_B Check Calcd Positive Resid. Density on Pd5_1 1.90 eA-3

Author Response: The large residual hole is around the Pd atoms center, probably due to difficulties in absorption correction.

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PLAT973_ALERT_2_B Check Calcd Positive Resid. Density on     Pd6_1       1.76 eA-3
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Author Response: The large residual hole is around the Pd atoms center, probably due to difficulties in absorption correction.

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PLAT973_ALERT_2_B Check Calcd Positive Resid. Density on     Pd4_1       1.75 eA-3
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Author Response: The large residual hole is around the Pd atoms center, probably due to difficulties in absorption correction.

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PLAT973_ALERT_2_B Check Calcd Positive Resid. Density on     Pd3_1       1.63 eA-3
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Author Response: The large residual hole is around the Pd atoms center, probably due to difficulties in absorption correction.

Alert level C

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RADNW01_ALERT_1_C  The radiation wavelength lies outside the expected range
           for the supplied radiation type. Expected range 0.71065-0.71075
           Wavelength given =    0.71000
PLAT026_ALERT_3_C Ratio Observed / Unique Reflections (too) Low ..        46% Check
PLAT077_ALERT_4_C Unit-Cell Contains Non-integer Number of Atoms .     Please Check
PLAT082_ALERT_2_C High R1 Value ..................................       0.14 Report
PLAT241_ALERT_2_C High  MainResAtom  Ueq as Compared to Neighbours      C38_2 Check
PLAT241_ALERT_2_C High  MainResAtom  Ueq as Compared to Neighbours      C32_3 Check
PLAT241_ALERT_2_C High  MainResAtom  Ueq as Compared to Neighbours       C4_4 Check
PLAT241_ALERT_2_C High  MainResAtom  Ueq as Compared to Neighbours      C32_4 Check
PLAT241_ALERT_2_C High  MainResAtom  Ueq as Compared to Neighbours      C32_5 Check
PLAT241_ALERT_2_C High  MainResAtom  Ueq as Compared to Neighbours       C3_6 Check
PLAT241_ALERT_2_C High  MainResAtom  Ueq as Compared to Neighbours       C3_7 Check
PLAT241_ALERT_2_C High  MainResAtom  Ueq as Compared to Neighbours      C32_7 Check
PLAT241_ALERT_2_C High  MainResAtom  Ueq as Compared to Neighbours      C38_7 Check
PLAT241_ALERT_2_C High  MainResAtom  Ueq as Compared to Neighbours      C31_8 Check
PLAT241_ALERT_2_C High  MainResAtom  Ueq as Compared to Neighbours      C32_8 Check
PLAT241_ALERT_2_C High  MainResAtom  Ueq as Compared to Neighbours      C37_8 Check
PLAT241_ALERT_2_C High  MainResAtom  Ueq as Compared to Neighbours      C39_8 Check
PLAT241_ALERT_2_C High  MainResAtom  Ueq as Compared to Neighbours      C38_9 Check
PLAT242_ALERT_2_C Low   MainResAtom  Ueq as Compared to Neighbours      Pd5_1 Check
PLAT242_ALERT_2_C Low   MainResAtom  Ueq as Compared to Neighbours      Pd6_1 Check
PLAT242_ALERT_2_C Low   MainResAtom  Ueq as Compared to Neighbours      C41_4 Check
PLAT242_ALERT_2_C Low   MainResAtom  Ueq as Compared to Neighbours      C30_8 Check
PLAT243_ALERT_4_C High MinorResAtom  Ueq as Compared to Neighbours      S2_15 Check
PLAT243_ALERT_4_C High MinorResAtom  Ueq as Compared to Neighbours      S2_16 Check
PLAT243_ALERT_4_C High MinorResAtom  Ueq as Compared to Neighbours      S2_17 Check
PLAT243_ALERT_4_C High MinorResAtom  Ueq as Compared to Neighbours      S2_20 Check
PLAT243_ALERT_4_C High MinorResAtom  Ueq as Compared to Neighbours      S2_21 Check
PLAT244_ALERT_4_C Low  MinorResAtom  Ueq as Compared to Neighbours      S2_18 Check
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PLAT244_ALERT_4_C Low  MinorResAtom  Ueq as Compared to Neighbours      S2_22 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including     Pd1_1      0.156 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including     F2_10      0.264 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including     F2_11      0.273 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including     F2_12      0.274 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including     F2_13      0.256 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including     F2_14      0.236 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including     S2_15      0.215 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including     S2_16      0.219 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including     S2_17      0.208 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including     S2_18      0.227 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including     S2_19      0.259 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including     S2_20      0.215 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including     S2_21      0.283 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including     S2_22      0.283 Check
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.01841 Ang.
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ...    -2.893 Report
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.500        96 Report
                  6  0  0,  -7  1  0,   4  2  0,   8  2  0,  13  2  0,  -5  4  0,
                 -3  4  0,   2  4  0,   1  6  0,   4  6  0,   3 12  0,  -2 -9  1,
                  0 -8  1,   1 -7  1,   0 -6  1,   1 -6  1,  -1 -5  1,   4 -5  1,
                  6 -5  1,  -3 -4  1,   7 -3  1,  -7 -1  1,  -4 -1  1,  -4  0  1,
                 17  8  1,  19  4  3,  17  8  5,  14 -9  7,  13 -8  7,   3  2  7,
                     (   66 More NOT listed: see .ckf listing file)
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .          1 Check
                  1  0  5,
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.04Ang From B1_14          2.11 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.23Ang From S2_20          1.51 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.96Ang From Pd6_1         -1.60 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H2_3      .     -0.32 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H3B_16    .     -0.39 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H3C_19    .     -0.41 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H4A_21    .     -0.31 eA-3
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Alert level G

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FORMU01_ALERT_2_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and the formula from the _atom_site* data.
           Atom count from _chemical_formula_sum:C280 H192 B4.6 F18.4 N24 O40 P8
           Atom count from the _atom_site data:  C279.6 H190.8 B4.6 F18.4 N24 O39
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
           symmetry error - see SYMMG tests
          From the CIF: _cell_formula_units_Z    2
          From the CIF: _chemical_formula_sum  C280 H192 B4.60 F18.40 N24 O40 P8
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          C         560.00    559.20    0.80
          H         384.00    381.60    2.40
          B           9.20      9.20    0.00
          F          36.80     36.80   -0.00
          N          48.00     48.00    0.00
          O          80.00     79.60    0.40
          P          16.00     16.00    0.00
          Pd         12.00     12.00    0.00
          S          16.00     15.60    0.40
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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite        385 Note
PLAT003_ALERT_2_G Number of Uiso or U(i,j)  Restrained non-H-Atoms        385 Report
PLAT041_ALERT_1_G Calc. and Reported SumFormula    Strings  Differ     Please Check
             Calc: C279.60 H190.80 B4.60 F18.40 N24 O39.80 P8 Pd6
                   S7.80
             Rep.: C280 H192 B4.60 F18.40 N24 O40 P8 Pd6 S8
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.30 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records         56 Report
PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records         84 Report
PLAT174_ALERT_4_G The CIF-Embedded .res File Contains FLAT Records         18 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          1 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records          2 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records          1 Report
PLAT244_ALERT_4_G Low  MinorResAtom  Ueq as Compared to Neighbours      B1_10 Check
PLAT244_ALERT_4_G Low  MinorResAtom  Ueq as Compared to Neighbours      B1_11 Check
PLAT244_ALERT_4_G Low  MinorResAtom  Ueq as Compared to Neighbours      B1_14 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F2_12      Constrained at        0.8 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F3_12      Constrained at        0.8 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F4_12      Constrained at        0.8 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F5_12      Constrained at        0.8 Check
PLAT300_ALERT_4_G Atom Site Occupancy of B1_12      Constrained at        0.8 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F2_13      Constrained at        0.8 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F3_13      Constrained at        0.8 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F4_13      Constrained at        0.8 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F5_13      Constrained at        0.8 Check
PLAT300_ALERT_4_G Atom Site Occupancy of B1_13      Constrained at        0.8 Check
PLAT300_ALERT_4_G Atom Site Occupancy of S2_19      Constrained at        0.8 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O1_19      Constrained at        0.8 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C3_19      Constrained at        0.8 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C4_19      Constrained at        0.8 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H3A_19     Constrained at        0.8 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H3B_19     Constrained at        0.8 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H3C_19     Constrained at        0.8 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H4A_19     Constrained at        0.8 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H4B_19     Constrained at        0.8 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H4C_19     Constrained at        0.8 Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd    4)        100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd    5)        100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd   11)        100% Note
PLAT432_ALERT_2_G Short Inter X...Y Contact  O29_3    ..C3_19    .        2.88 Ang.
                                                     x,y,z  =      1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  O28_7    ..C4_19    .        2.92 Ang.
                                                     x,y,z  =      1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  O29_8    ..C4_21    .        2.76 Ang.
                                                     x,y,z  =      1_555 Check
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in  Crystal Structure          ! Info
PLAT790_ALERT_4_G Centre of Gravity not Within Unit-Cell: Resd.  #          3 Note
             B F4
PLAT790_ALERT_4_G Centre of Gravity not Within Unit-Cell: Resd.  #          4 Note
             B F4
PLAT790_ALERT_4_G Centre of Gravity not Within Unit-Cell: Resd.  #          5 Note
             B F4
PLAT790_ALERT_4_G Centre of Gravity not Within Unit-Cell: Resd.  #          6 Note
             B F4
PLAT794_ALERT_5_G Tentative Bond Valency for Pd1_1     (II)      .        2.22 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Pd2_1     (II)      .        2.33 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Pd4_1     (II)      .        2.25 Info
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PLAT794_ALERT_5_G Tentative Bond Valency for Pd5_1     (II)      .       2.19 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Pd6_1     (II)      .       2.23 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............      7414 Note
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE  Suppressed         ! Info
PLAT910_ALERT_3_G Missing FCF Reflection(s) Below Theta(Min)[Deg]=      0.84 Note
                0  1  0,   0  0  1,
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File        24 Note
                6  0  0,  -7  1  0,   4  2  0,   8  2  0,  13  2  0,  -5  4  0,
               -3  4  0,   2  4  0,   1  6  0,   4  6  0,   3 12  0,  -2 -9  1,
                0 -8  1,   1 -7  1,   0 -6  1,   1 -6  1,  -1 -5  1,   4 -5  1,
                6 -5  1,  -3 -4  1,   7 -3  1,  -7 -1  1,  -4 -1  1,  -4  0  1,
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........     5.481 Note
            Predicted wR2: Based on SigI**2  9.56 or SHELX Weight 39.90
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         0 Info
PLAT994_ALERT_1_G SHELXL .ins Contains no or MERG 0 Instruction ..         ! Note
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   4 ALERT level A = Most likely a serious problem - resolve or explain
   4 ALERT level B = A potentially serious problem, consider carefully
  54 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  59 ALERT level G = General information/check it is not something unexpected

   5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  55 ALERT type 2 Indicator that the structure model may be wrong or deficient
   9 ALERT type 3 Indicator that the structure quality may be low
  46 ALERT type 4 Improvement, methodology, query or suggestion
   6 ALERT type 5 Informative message, check
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It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

PLATON version of 15/01/2026; check.def file version of 02/01/2026

Datablock mhw01_sq - ellipsoid plot