checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mhw02_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: mhw02_sq

Bond precision: C-C = 0.0085 A Wavelength=1.34135

Cell: a=27.629(3) b=27.629(3) c=48.349(6)
alpha=90 beta=90 gamma=120
Temperature: 193 K

	Calculated	Reported
Volume	31963(8)	31963(8)
Space group	P 31 2 1	P 31 2 1
Hall group	P 31 2"	P 31 2"
Moiety formula	C264 H144 N24 O32 P8 Pd6, 10.2(B F4), 6(C2 H3 N) [+ solvent]	?
Sum formula	C276 H162 B10.20 F40.80 N30 O32 P8 Pd6 [+ solvent]	C276 H162 B10.20 F40.80 N30 O32 P8 Pd6
Mr	6181.99	6181.97
Dx,g cm-3	0.964	0.963
Z	3	3
Mu (mm-1)	1.904	1.904
F000	9294.6	9295.0
F000'	9324.94	
h,k,lmax	33,33,58	33,33,58
Nref	39397[21005]	39193
Tmin,Tmax	0.717,0.683	0.578,0.751
Tmin'	0.651	

Correction method= # Reported T Limits: Tmin=0.578 Tmax=0.751
AbsCorr = MULTI-SCAN

Data completeness= 1.87/0.99 Theta(max)= 54.114

R(reflections)= 0.0401(33259) wR2(reflections)= 0.1196(39193)

S = 1.030 Npar= 1860

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 C

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PLAT077_ALERT_4_C Unit-Cell Contains Non-integer Number of Atoms .     Please Check
PLAT241_ALERT_2_C High  MainResAtom  Ueq as Compared to Neighbours       C3_2 Check
PLAT241_ALERT_2_C High  MainResAtom  Ueq as Compared to Neighbours      C32_2 Check
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       C3_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      C38_4 Check
PLAT241_ALERT_2_C High  MainResAtom  Ueq as Compared to Neighbours      C32_5 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including      F2_6      0.247 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including      F2_7      0.246 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including      F2_8      0.240 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including      F2_9      0.257 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including     F2_10      0.228 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including     F2_11      0.280 Check
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.00847 Ang.
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600        38 Report
                  0  3  0,   0  4  0,  -2  5  0,   0  5  0,   0  7  0,  -1  1  1,
                  0  1  1,  -3  3  1,   0  3  1,  -2  3  2,  -1  3  2,   0  4  2,
                  0  0  3,  -3  3  3,  -2  4  3,   0  8  3,  -2  2  4,   0  2  4,
                 -5  5  4,   0  5  4,   0  1  5,  -1  2  5,  -6  6  7,  -3  3  8,
                 -4  4  8,   0 13  8,  -1  1  9,   0  1  9,  -2  7  9,  -8  8  9,
                     (    8 More NOT listed: see .ckf listing file)
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Alert level G

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ABSMU01_ALERT_1_G  Calculation of _exptl_absorpt_correction_mu
                   not performed for this radiation type.
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite        42 Note
PLAT003_ALERT_2_G Number of Uiso or U(i,j)  Restrained non-H-Atoms        30 Report
PLAT033_ALERT_4_G Flack x Value Deviates > 3.0 * Sigma from Zero .     0.057 Note
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records         6 Report
PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records         7 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         1 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_6 Check
PLAT244_ALERT_4_G Low  MinorResAtom  Ueq as Compared to Neighbours       B1_8 Check
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PLAT244_ALERT_4_G Low  MinorResAtom  Ueq as Compared to Neighbours      B1_11 Check
PLAT299_ALERT_4_G Atom Site Occupancy Constrained at .............        0.5 Check
             F2_10   F3_10   F4_10   F5_10   B1_10   H15A_13 H15B_13 H15C_13
             H3A_14  H3B_14  H3C_14
PLAT300_ALERT_4_G Atom Site Occupancy of F2_7       Constrained at        0.8 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F3_7       Constrained at        0.8 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F4_7       Constrained at        0.8 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F5_7       Constrained at        0.8 Check
PLAT300_ALERT_4_G Atom Site Occupancy of B1_7       Constrained at        0.8 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F2_9       Constrained at        0.8 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F3_9       Constrained at        0.8 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F4_9       Constrained at        0.8 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F5_9       Constrained at        0.8 Check
PLAT300_ALERT_4_G Atom Site Occupancy of B1_9       Constrained at        0.8 Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd    3)       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    6)       100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    6)       2.50 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.  #          7 Note
             B F4
PLAT794_ALERT_5_G Tentative Bond Valency for Pd1_1     (II)      .       2.27 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Pd2_1     (II)      .       2.24 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Pd3_1     (II)      .       2.23 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Pd4_1     (II)      .       2.22 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        576 Note
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE  Suppressed          ! Info
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         64 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....          2 Note
              -1  1  1,   0  1  1,
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File         52 Note
                2  3  0,   0  4  0,  -2  5  0,   2  5  0,   0  7  0,   0  3  1,
              -10  7  1,  -3  2  2,   1  2  2,  -2  3  2,  -1  3  2,  -3  3  3,
                0  2  4,  -3  6  4,   0  1  5,   2  3  5,  -1  1  9,   0  1  9,
               -2  7  9,  -8  8  9,  -7  7 10,   1  1 11,  -1  2 11,   0  4 11,
               -3  3  1,  -3 10  1,   0  8  3,  -2  2  4,  -5  5  4,  -1  2  6,
               -6  6  7,  -3  3  8,  -4  4  8,   0 13  8,   2  5  9,   1  3 12,
                1  1 13,  -5  5 18,   0  5 18,   0  3  0,   0  4  2,   2  2  3,
               -2  4  3,   0  5  4,   1  3 11,  -3  4 11,  -1  4 12,  -1  3  0,
               -1  2  5,   0  2 12,
                   (    2 More NOT listed: see .ckf listing file)
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........      4.004 Note
             Predicted wR2: Based on SigI**2  2.99 or SHELX Weight 11.74
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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   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
  17 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  41 ALERT level G = General information/check it is not something unexpected

   2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  18 ALERT type 2 Indicator that the structure model may be wrong or deficient
   4 ALERT type 3 Indicator that the structure quality may be low
  29 ALERT type 4 Improvement, methodology, query or suggestion
   5 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 mhw02_sq - ellipsoid plot