checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mhw03_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: mhw03_sq

Bond precision: C-C = 0.0224 A Wavelength=0.71073

Cell: a=34.9006(7) b=34.9006(7) c=56.377(2)
alpha=90 beta=90 gamma=90
Temperature: 193 K

	Calculated	Reported
Volume	68670(4)	68670(4)
Space group	P 43	P 43
Hall group	P 4cw	P 4cw
Moiety formula	2(C264 H144 N24 O32 P8 Pd6), 5(B F4), 12(C2 H3 N) [+ solvent]	?
Sum formula	C552 H324 B5 F20 N60 O64 P16 Pd12 [+ solvent]	C552 H324 B5 F20 N60 O64 P16 Pd12
Mr	11026.99	11027.06
Dx,g cm-3	1.067	1.067
Z	4	4
Mu (mm-1)	0.406	0.406
F000	22260.0	22260.0
F000'	22228.18	
h,k,lmax	42,42,68	42,42,68
Nref	128109[64758]	126434
Tmin,Tmax	0.922,0.922	0.544,0.753
Tmin'	0.922	

Correction method= # Reported T Limits: Tmin=0.544 Tmax=0.753
AbsCorr = MULTI-SCAN

Data completeness= 1.95/0.99 Theta(max)= 25.515

R(reflections)= 0.1331(99350) wR2(reflections)= 0.3486(126434)

S = 1.176 Npar= 6562

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 B

PLAT342_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.02238 Ang.

Author Response: The flexibility of the modelled structure is reflected in the low precision of C-C bonds.

Alert level C

RINTA01_ALERT_3_C The value of Rint is greater than 0.12
Rint given 0.150

PLAT020_ALERT_3_C	The Value of Rint is Greater Than 0.12	0.150 Report
PLAT082_ALERT_2_C	High R1 Value	0.13 Report
PLAT084_ALERT_3_C	High wR2 Value (i.e. > 0.25)	0.35 Report
PLAT241_ALERT_2_C	High MainResAtom Ueq as Compared to Neighbours	O27_2 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	C38_2 Check
PLAT241_ALERT_2_C	High MainResAtom Ueq as Compared to Neighbours	C31_3 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_5 Check
PLAT241_ALERT_2_C	High MainResAtom Ueq as Compared to Neighbours	C15_6 Check
PLAT241_ALERT_2_C	High MainResAtom Ueq as Compared to Neighbours	C32_6 Check
PLAT241_ALERT_2_C	High MainResAtom Ueq as Compared to Neighbours	C39_6 Check
PLAT241_ALERT_2_C	High MainResAtom Ueq as Compared to Neighbours	C31_7 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	C4_9 Check
PLAT241_ALERT_2_C	High MainResAtom Ueq as Compared to Neighbours	C32_9 Check
PLAT241_ALERT_2_C	High MainResAtom Ueq as Compared to Neighbours	O28_11 Check
PLAT241_ALERT_2_C	High MainResAtom Ueq as Compared to Neighbours	O28_13 Check
PLAT241_ALERT_2_C	High MainResAtom Ueq as Compared to Neighbours	O13_14 Check
PLAT241_ALERT_2_C	High MainResAtom Ueq as Compared to Neighbours	O28_14 Check
PLAT241_ALERT_2_C	High MainResAtom Ueq as Compared to Neighbours	O28_16 Check
PLAT241_ALERT_2_C	High MainResAtom Ueq as Compared to Neighbours	N34_18 Check
PLAT241_ALERT_2_C	High MainResAtom Ueq as Compared to Neighbours	C23_11 Check
PLAT241_ALERT_2_C	High MainResAtom Ueq as Compared to Neighbours	C37_11 Check
PLAT241_ALERT_2_C	High MainResAtom Ueq as Compared to Neighbours	C12_12 Check
PLAT241_ALERT_2_C	High MainResAtom Ueq as Compared to Neighbours	C9_13 Check
PLAT241_ALERT_2_C	High MainResAtom Ueq as Compared to Neighbours	C32_13 Check

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PLAT241_ALERT_2_C High  MainResAtom  Ueq as Compared to Neighbours     C15_14 Check
PLAT241_ALERT_2_C High  MainResAtom  Ueq as Compared to Neighbours     C32_14 Check
PLAT241_ALERT_2_C High  MainResAtom  Ueq as Compared to Neighbours     C38_14 Check
PLAT241_ALERT_2_C High  MainResAtom  Ueq as Compared to Neighbours      C3_15 Check
PLAT241_ALERT_2_C High  MainResAtom  Ueq as Compared to Neighbours     C23_15 Check
PLAT241_ALERT_2_C High  MainResAtom  Ueq as Compared to Neighbours     C37_15 Check
PLAT241_ALERT_2_C High  MainResAtom  Ueq as Compared to Neighbours     C23_16 Check
PLAT241_ALERT_2_C High  MainResAtom  Ueq as Compared to Neighbours     C31_17 Check
PLAT241_ALERT_2_C High  MainResAtom  Ueq as Compared to Neighbours      C4_18 Check
PLAT241_ALERT_2_C High  MainResAtom  Ueq as Compared to Neighbours     C15_18 Check
PLAT242_ALERT_2_C Low   MainResAtom  Ueq as Compared to Neighbours      Pd2_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      C30_3 Check
PLAT242_ALERT_2_C Low   MainResAtom  Ueq as Compared to Neighbours       C7_4 Check
PLAT242_ALERT_2_C Low   MainResAtom  Ueq as Compared to Neighbours      C18_5 Check
PLAT242_ALERT_2_C Low   MainResAtom  Ueq as Compared to Neighbours      C16_6 Check
PLAT242_ALERT_2_C Low   MainResAtom  Ueq as Compared to Neighbours      C26_8 Check
PLAT242_ALERT_2_C Low   MainResAtom  Ueq as Compared to Neighbours      N1_17 Check
PLAT243_ALERT_4_C High MinorResAtom  Ueq as Compared to Neighbours      C2_28 Check
PLAT244_ALERT_4_C Low  MinorResAtom  Ueq as Compared to Neighbours      C2_26 Check
PLAT244_ALERT_4_C Low  MinorResAtom  Ueq as Compared to Neighbours      C2_27 Check
PLAT244_ALERT_4_C Low  MinorResAtom  Ueq as Compared to Neighbours      C2_29 Check
PLAT244_ALERT_4_C Low  MinorResAtom  Ueq as Compared to Neighbours      C2_33 Check
PLAT244_ALERT_4_C Low  MinorResAtom  Ueq as Compared to Neighbours      C2_35 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including     F2_19      0.144 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including     F2_20      0.149 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including     F2_21      0.133 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including     F2_34      0.166 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including     F2_36      0.165 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including     N1_26      0.122 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including     N1_28      0.112 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including     N1_29      0.135 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including     N1_35      0.107 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600          9 Report
               -1  6  0,   1  6  0,   5  8  0,  -1  3  2,   1  3  2,   0  0  4,
                0  2  4,   3  3  6,   1  3 21,
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF ....          5 Note
               -1  3  2,   1  3  2,   0  0  4,   0  2  4,   3  3  6,
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.77Ang From Pd4_1          -1.91 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.56Ang From Pd6_1          -1.85 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.59Ang From Pd6_1          -1.80 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.68Ang From Pd5_10         -1.70 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.51Ang From Pd5_1          -1.69 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.56Ang From Pd1_1          -1.60 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.61Ang From Pd3_10         -1.60 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.66Ang From Pd3_10         -1.51 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H37_3     .      -0.36 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H16_4     .      -0.31 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H38_4     .      -0.41 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H41_5     .      -0.31 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H9_6      .      -0.49 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H8_8      .      -0.33 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H31_9     .      -0.37 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H39_9     .      -0.33 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H8_12     .      -0.35 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H16_14    .      -0.34 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H35_15    .      -0.49 eA-3
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PLAT977_ALERT_2_C Check Negative Difference Density on H39_16    .      -0.57 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H23_17    .      -0.62 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H3A_23    .      -0.31 eA-3
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Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite        717 Note
PLAT003_ALERT_2_G Number of Uiso or U(i,j)  Restrained non-H-Atoms        717 Report
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.25 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records         58 Report
PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records         85 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
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_19 Check
PLAT244_ALERT_4_G Low  MinorResAtom  Ueq as Compared to Neighbours      B1_20 Check
PLAT244_ALERT_4_G Low  MinorResAtom  Ueq as Compared to Neighbours      B1_21 Check
PLAT244_ALERT_4_G Low  MinorResAtom  Ueq as Compared to Neighbours      B1_34 Check
PLAT244_ALERT_4_G Low  MinorResAtom  Ueq as Compared to Neighbours      B1_36 Check
PLAT344_ALERT_2_G Unusual sp?       Angle Range in Solvent/Ion for      C2_28 Check
PLAT367_ALERT_2_G Long?  C(sp?)-C(sp?) Bond  C2_28    - C3_28    .       1.52 Ang.
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in  Crystal Structure          ! Info
PLAT608_ALERT_4_G ADDSYM Test Skipped (Too Time-consuming) .......          ! Info
PLAT794_ALERT_5_G Tentative Bond Valency for Pd1_1     (II)      .       2.30 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Pd2_1     (II)      .       2.25 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)      .       2.37 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Pd5_1     (II)      .       2.18 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Pd6_1     (II)      .       2.46 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Pd1_10    (II)      .       2.25 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Pd2_10    (II)      .       2.27 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Pd3_10    (II)      .       2.19 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Pd4_10    (II)      .       2.29 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Pd5_10    (II)      .       2.36 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Pd6_10    (II)      .       2.26 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............      13489 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]=       0.83 Note
                  0  1  0,   0  1  1,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        239 Note
PLAT916_ALERT_2_G Hooft y and Flack x Parameter Values Differ by .       0.25 Check
PLAT930_ALERT_2_G FCF-based   Twin Law ( 1 0 0)         Est.d BASF       0.29 Check
PLAT931_ALERT_5_G CIFcalcFCF  Twin Law ( 1 0 0)         Est.d BASF       0.36 Check
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File         24 Note
                  1  8-27,   1  6-26,   3  9-26,   7 11-26,   8 10-25,   7 11-24,
                  2  6-23,   7 12-23,  -2  3-22,   1  2-21,   1  3-21,  -1  4-20,
                  1  7-20, -10 11-20,   3 11-20, -16 20-20,  -1  4-19,   2  6-19,
                  3 11-18,   1  7-17,  -1  3-16,  -4  5-16,   7  9-16,  -1 10-16,
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........       4.353 Note
              Predicted wR2: Based on SigI**2  8.01 or SHELX Weight 30.05
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
  1 ALERT level B = A potentially serious problem, consider carefully
 85 ALERT level C = Check. Ensure it is not caused by an omission or oversight
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 40 ALERT level G = General information/check it is not something unexpected

  1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 83 ALERT type 2 Indicator that the structure model may be wrong or deficient
  8 ALERT type 3 Indicator that the structure quality may be low
 20 ALERT type 4 Improvement, methodology, query or suggestion
 14 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 mhw03_sq - ellipsoid plot