

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: hh

Bond precision:	C-C = 0.0117 A	Wavelength=0.71073
Cell:	a=17.5839(13) b=17.1893(10) c=21.0431(15)	alpha=90 beta=107.029(2) gamma=90
Temperature:	150 K	
	Calculated	Reported
Volume	6081.5(7)	6081.5(7)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C47.69 H95.08 Mn4 O16, 0.306(C H3)	C40 H72 Mn4 O12, 4(C2 H6 O)
Sum formula	C48 H96 Mn4 O16	C48 H96 Mn4 O16
Mr	1149.01	1149.00
Dx, g cm ⁻³	1.255	1.255
Z	4	4
Mu (mm ⁻¹)	0.869	0.869
F000	2448.0	2448.0
F000'	2454.40	
h, k, lmax	21, 20, 25	21, 20, 25
Nref	11149	11115
Tmin, Tmax	0.901, 0.941	0.633, 0.745
Tmin'	0.885	

Correction method= # Reported T Limits: Tmin=0.633 Tmax=0.745
AbsCorr = NONE

Data completeness= 0.997 Theta(max) = 25.356

R(reflections)= 0.0708(6251)

wR2(reflections)=
0.2098(11115)

S = 1.043

Npar= 807

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**

RINTA01_ALERT_3_C The value of Rint is greater than 0.12
Rint given 0.125

PLAT020_ALERT_3_C The Value of Rint is Greater Than 0.12 0.125 Report

PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ Please Check
Calc: C47.69 H95.08 Mn4 O16, 0.306(C H3)
Rep.: C40 H72 Mn4 O12, 4(C2 H6 O)

PLAT234_ALERT_4_C Large Hirshfeld Difference O3 --C58 . 0.17 Ang.

PLAT234_ALERT_4_C Large Hirshfeld Difference C2 --C22 . 0.16 Ang.

PLAT234_ALERT_4_C Large Hirshfeld Difference C40 --C41 . 0.18 Ang.

PLAT234_ALERT_4_C Large Hirshfeld Difference C40 --C43 . 0.16 Ang.

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C22 Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C40 Check

PLAT260_ALERT_2_C Large Average Ueq of Residue Including C9 0.123 Check

PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds 0.01167 Ang.

PLAT360_ALERT_2_C Short C(sp3)-C(sp3) Bond C34 - C56 . 1.43 Ang.

PLAT360_ALERT_2_C Short C(sp3)-C(sp3) Bond C58 - C63 . 1.37 Ang.

● **Alert level G**

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 37 Report

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 7 Report
H2AA H3 H7 H13 H2BB H9 H15

PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 7.50 Why ?

PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 6 Report

PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used 0.0100 Report

PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used 0.0100 Report

PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used 0.0010 Report

PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used 0.0100 Report

PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used 0.0100 Report

PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used 0.0100 Report

PLAT301_ALERT_3_G Main Residue Disorder(Resd 1) 25% Note

PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2) 100% Note

PLAT304_ALERT_4_G Non-Integer Number of Atoms in (Resd 1) 162.78 Check

PLAT304_ALERT_4_G Non-Integer Number of Atoms in (Resd 2) 1.22 Check

PLAT367_ALERT_2_G Long? C(sp?)-C(sp?) Bond C36 - C60 . 1.53 Ang.

PLAT412_ALERT_2_G Short Intra XH3 .. XHn H10 ..H51B . 2.00 Ang.
x,y,z = 1_555 Check

PLAT412_ALERT_2_G Short Intra XH3 .. XHn H24A ..H7B . 2.12 Ang.
x,y,z = 1_555 Check

PLAT412_ALERT_2_G Short Intra XH3 .. XHn H27A ..H44 . 1.99 Ang.
x,y,z = 1_555 Check

PLAT412_ALERT_2_G Short Intra XH3 .. XHn H46 ..H43C . 1.86 Ang.
x,y,z = 1_555 Check

PLAT413_ALERT_2_G Short Inter XH3 .. XHn H48B ..H43B . 2.12 Ang.
2-x,1-y,1-z = 3_766 Check

PLAT414_ALERT_2_G Short Intra D-H..H-X H30A ..H15 . 2.13 Ang.
x,y,z = 1_555 Check

PLAT432_ALERT_2_G Short Inter X...Y Contact O19 ..C9 . 2.88 Ang.
x,y,z = 1_555 Check

PLAT432_ALERT_2_G Short Inter X...Y Contact C36 ..C9 . 2.62 Ang.

PLAT432_ALERT_2_G Short Inter X...Y Contact	C60	x,y,z =	1_555 Check
		..C9	1.81 Ang.
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels	x,y,z =	1_555 Check
	H2AA H2BB		2 Note
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C9	--C60		1.80 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C25	--C28		1.75 Ang.
PLAT860_ALERT_3_G Number of Least-Squares Restraints		378 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary	.		Please Do !
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity		3.4 Low

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
13 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
30 **ALERT level G** = General information/check it is not something unexpected

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
19 ALERT type 2 Indicator that the structure model may be wrong or deficient
12 ALERT type 3 Indicator that the structure quality may be low
9 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

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. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 06/01/2024; check.def file version of 05/01/2024

Datablock hh - ellipsoid plot

