

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 = 0.0058 A	Wavelength=0.71073	
Cell:	a=10.621(2)	b=13.017(3)	c=19.727(5)
	alpha=77.996(5)	beta=88.842(4)	gamma=67.691(4)
Temperature:	150 K		
	Calculated	Reported	
Volume	2462.8(10)	2462.8(10)	
Space group	P -1	P -1	
Hall group	-P 1	-P 1	
Moiety formula	C38 H68 Mn2 O10, C3 H8 O	C38 H68 Mn2 O10, C3 H8 O	
Sum formula	C41 H76 Mn2 O11	C41 H76 Mn2 O11	
Mr	854.90	854.89	
Dx, g cm-3	1.153	1.153	
Z	2	2	
Mu (mm-1)	0.562	0.562	
F000	920.0	920.0	
F000'	921.74		
h, k, lmax	12, 15, 23	12, 14, 22	
Nref	8774	7479	
Tmin, Tmax	0.924, 0.945	0.602, 0.745	
Tmin'	0.924		

Correction method= # Reported T Limits: Tmin=0.602 Tmax=0.745
AbsCorr = NONE

Data completeness= 0.852 Theta(max)= 25.098

R(reflections)= 0.0455(5753)

wR2(reflections)=
0.1465(7479)

S = 1.077

Npar= 591

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**

PLAT029_ALERT_3_B _diffn_measured_fraction_theta_full value Low . 0.956 Why?

Author Response: A full set of data was collected, however some bad reflections were removed by omit command resulting in a relatively low data completeness of 95.6%. Data-to-parameter ratio is more than 12, and intensity to noise ratio is higher than 15, which are good enough to guarantee a reliable structure refinement.

● **Alert level C**

PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.7 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference C17 --C4A . 0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C17 --C5A . 0.19 Ang.
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C17 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C26 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C28 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C31 Check

● **Alert level G**

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 21 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 1 Report
H00C
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 3 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
PLAT230_ALERT_2_G Hirshfeld Test Diff for C17 --C6A . 7.5 s.u.
PLAT301_ALERT_3_G Main Residue Disorder(Resd 1) 18% Note
PLAT412_ALERT_2_G Short Intra XH3 .. XHn H2AA ..H11 . 2.03 Ang.
x,y,z = 1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn H19 ..H5AB . 1.99 Ang.
x,y,z = 1_555 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 40 Note
O00C H00C C00P H00P C011 C012 H01A H01B
H01C C018 H01D H01E H01F H2AA H2AB H2AC
H1AA H1AB H1AC H3AA H3AB H3AC H7AA H7AB
H7AC H9AA H9AB H9AC H8AA H8AB H8AC H5AA
H5AB H5AC H6AA H6AB H6AC H4AA H4AB H4AC
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C011 --C2 1.74 Ang.
PLAT794_ALERT_5_G Tentative Bond Valency for Mn1 (II) . 2.19 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Mn2 (II) . 2.18 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints 198 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 47 Note
1 1 1, 2 0 6, 2 1 7, 1 0 9, 3 2 5, 2 0 13,

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-5 -7 5, 4 1 4, -2 -4 12, -1 -2 5, 1 0 6, -1 -3 12,
2 1 14, -6 -8 3, 1 0 13, -4 -7 7, -3 -5 8, 0 -2 6,
-3 -5 11, -5 -7 7, -3 -5 7, 6 6 9, 1 0 7, 1 -1 6,
-6 -8 2, -4 -6 8, -2 -4 11, -1 -2 4, 0 -2 13, -1 -3 13,
-1 -3 11, -3 -6 9, -5 -7 4, 2 0 14, -4 -6 7, 0 -1 7,
4 5 0, 1 -1 14, -3 -4 2, -3 -5 9, 1 0 8, -1 -3 5,
4 3 2, 5 5 12, -4 -7 8, 0 -1 5, -4 -6 5,

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PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 1.4 Low

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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
7 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
18 **ALERT level G** = General information/check it is not something unexpected
- 1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
11 ALERT type 2 Indicator that the structure model may be wrong or deficient
7 ALERT type 3 Indicator that the structure quality may be low
4 ALERT type 4 Improvement, methodology, query or suggestion
3 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. 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.

