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.

Datablock: d

Bond precision:	C-C = 0.0042 A	Wavelength=0.71073	
Cell:	a=9.2163(18)	b=13.278(3)	c=17.365(4)
	alpha=90	beta=95.41(3)	gamma=90
Temperature:	293 К		
	Calculated	Reporte	ed
Volume	2115.6(8)	2115.6	(7)
Space group	P 21/n	P 21/n	
Hall group	-P 2yn	−P 2yn	
Moiety formula	C12 H23 C14 Mn2 N	05 ?	
Sum formula	C12 H23 C14 Mn2 N	O5 C12 H23	3 Cl4 Mn2 N O5
Mr	512.99	512.99	
Dx,g cm-3	1.611	1.611	
Z	4	4	
Mu (mm-1)	1.718	1.718	
F000	1040.0	1040.0	
F000'	1045.37		
h,k,lmax	11,16,21	11,16,2	21
Nref	4366	4337	
Tmin, Tmax	0.741,0.842	0.453,3	1.000
Tmin'	0.644		
Correction method AbsCorr = MULTI-	od= # Reported T Lin -SCAN	nits: Tmin=0.453	Tmax=1.000
Data completenes	ss= 0.993	Theta(max) = 26.	. 448
R(reflections)=	0.0324(3585)		wR2(reflections) = 0.0923(4337)
S = 1.130	Npar= 22	Λ	0.0323(4337)
2 1.100	MPGI 22	•	

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

PLAT018_ALERT_1_C _diffrn_measured_fraction_theta_max .NE. *_full ! Check PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Mn1 Check PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Mn2 Check

Alert level G

PLAT013_ALERT_1_G N.O.Kshelx_hkl_checksum Found in CIF	Please Check
PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K)	293 Check
PLAT200_ALERT_1_G Reporteddiffrn_ambient_temperature (K)	293 Check
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Mn1C13 .	10.8 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Mn1O10 .	5.5 s.u.
PLAT794_ALERT_5_G Tentative Bond Valency for Mn1 (II) .	2.20 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Mn2 (II) .	2.12 Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .	Please Do !
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged	Please Check

- 0 ALERT level A = Most likely a serious problem resolve or explain
- 0 ALERT level B = A potentially serious problem, consider carefully
- 3 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
- 9 **ALERT level G** = General information/check it is not something unexpected
- 5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
- 5 ALERT type 2 Indicator that the structure model may be wrong or deficient
- 0 ALERT type 3 Indicator that the structure quality may be low
- O ALERT type 4 Improvement, methodology, query or suggestion
- 2 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 28/11/2022; check.def file version of 28/11/2022

