

## 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: shelx

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Bond precision:	As- O = 0.0015 A	Wavelength=0.71073
Cell:	a=8.8761 (1)	b=7.5190 (8)      c=11.6890 (12)
	alpha=90	beta=90      gamma=90
Temperature:	293 K	
	Calculated	Reported
Volume	780.12 (12)	780.12 (12)
Space group	P b c m	P b c m
Hall group	-P 2c 2b	-P 2c 2b
Moiety formula	As <sub>8</sub> H <sub>4</sub> Mg <sub>0.78</sub> Mn <sub>7.22</sub> O <sub>40</sub> , 4.616 (Ca), 3.384 (Na)	?
Sum formula	As <sub>8</sub> Ca <sub>4.62</sub> H <sub>4</sub> Mg <sub>0.78</sub> Mn <sub>7.22</sub> Na <sub>3.38</sub> O <sub>40</sub>	As <sub>8</sub> Ca <sub>4.62</sub> H <sub>4</sub> Mg <sub>0.78</sub> Mn <sub>7.22</sub> Na <sub>3.38</sub> O <sub>40</sub>
Mr	1921.71	1921.71
Dx, g cm <sup>-3</sup>	4.090	4.090
Z	1	1
Mu (mm <sup>-1</sup> )	12.220	12.220
F000	907.4	907.4
F000'	911.85	
h, k, lmax	14, 12, 19	14, 12, 19
Nref	1931	1885
Tmin, Tmax	0.562, 0.652	0.576, 0.664
Tmin'	0.372	

Correction method= # Reported T Limits: Tmin=0.576 Tmax=0.664

AbsCorr = MULTI-SCAN

Data completeness= 0.976

Theta (max)= 36.048

R(reflections)= 0.0250( 1554)

wR2(reflections)=  
0.0508( 1885)

S = 1.113

Npar= 88

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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

PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms ..	Please Check
PLAT220_ALERT_2_C NonSolvent Resd 1 O Ueq(max)/Ueq(min) Range	3.6 Ratio



#### Alert level G

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension	2 Info
PLAT168_ALERT_4_G The CIF-Embedded .res File Contains EXYZ Records	3 Report
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records	3 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)	293 Check
PLAT200_ALERT_1_G Reported _diffn_ambient_temperature ..... (K)	293 Check
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1 )	12% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2 )	100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 3 )	100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 4 )	100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 5 )	100% Note
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

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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  
2 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
12 **ALERT level G** = General information/check it is not something unexpected

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

