checkCIF/PLATON report

Structure factors have been supplied for datablock(s) FCHMAG_1_0m

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: FCHMAG_1_0m

```
Bond precision:   As- O = 0.0010 A         Wavelength=0.71073

Cell:              a=19.7144(5)      b=19.7144(5)      c=19.7144(5)
                   alpha=90          beta=90           gamma=90
Temperature:       293 K
```

	Calculated	Reported
Volume	7662.2(6)	7662.2(6)
Space group	I a -3 d	I a -3 d
Hall group	-I 4bd 2c 3	-I 4bd 2c 3
Moiety formula	As96 Mn146.50 O288, 0.264(O48), 0.113(O48)	?
Sum formula	As96 Mn146.50 O306.10	As96 Mn146.50 O306.10
Mr	20138.52	20138.91
Dx,g cm-3	4.364	4.365
Z	1	1
Mu (mm-1)	16.203	16.203
F000	9279.2	9279.0
F000'	9338.49	
h,k,lmax	30,30,30	30,30,30
Nref	1267	1241
Tmin,Tmax	0.105,0.327	0.528,0.747
Tmin'	0.079	

```
Correction method= # Reported T Limits: Tmin=0.528 Tmax=0.747
AbsCorr = MULTI-SCAN

Data completeness= 0.979           Theta(max)= 33.469

R(reflections)= 0.0119( 1093)                    wR2(reflections)=
                                                 0.0256( 1241)
S = 1.070                  Npar= 72
```

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

```
PLAT212_ALERT_2_B ADP of Atom ClW2      is N.P.D. or (nearly) 2D .     Please Check
PLAT220_ALERT_2_B NonSolvent   Resd 1 Mn   Ueq(max)/Ueq(min) Range        6.3 Ratio
```

Alert level C

```
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         19 Report
PLAT976_ALERT_2_C Check Calcd Resid. Dens.  0.70Ang From O1      .      -0.41 eA-3
```

Alert level G

```
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          2 Info
PLAT017_ALERT_1_G Check Scattering Type Consistency of MX       as         MN
PLAT017_ALERT_1_G Check Scattering Type Consistency of CLW1     as         O
PLAT017_ALERT_1_G Check Scattering Type Consistency of CLW2     as         O
PLAT019_ALERT_1_G _diffrn_measured_fraction_theta_full/*_max < 1.0      0.989 Report
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)...     Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large       7.60 Why ?
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)        293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)        293 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )        22% 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
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........          3 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600          4 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File         19 Note
```

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

   7 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
   2 ALERT type 3 Indicator that the structure quality may be low
   4 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
```

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PLAT212_FCHMAG_1_0m
;
PROBLEM: ADP of Atom ClW2      is N.P.D. or (nearly) 2D .     Please Check
RESPONSE: ...
;
```

```
_vrf_PLAT220_FCHMAG_1_0m
;
PROBLEM: NonSolvent   Resd 1 Mn   Ueq(max)/Ueq(min) Range        6.3 Ratio
RESPONSE: ...
;
_vrf_PLAT911_FCHMAG_1_0m
;
PROBLEM: Missing FCF Refl Between Thmin & STh/L=    0.600         19 Report
RESPONSE: ...
;
_vrf_PLAT976_FCHMAG_1_0m
;
PROBLEM: Check Calcd Resid. Dens.  0.70Ang From O1      .      -0.41 eA-3
RESPONSE: ...
;
# end Validation Reply Form
```

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 18/05/2022; check.def file version of 17/05/2022

Datablock FCHMAG_1_0m - ellipsoid plot