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: I

Bond precision: C-C = 0.0084 A Wavelength=0.71073

Cell: a=13.4241(18) b=14.2981(19) c=20.254(3)
alpha=95.073(3) beta=99.802(2) gamma=93.632(2)
Temperature: 293 K

	Calculated	Reported
Volume	3803.6(9)	3803.5(9)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C36 H29 Mn N10 S2, C36 H28 Mn N10 S2, C3 H7 N O, O	C37.5 H34.5 Mn N10.5 O1.5 S2
Sum formula	C75 H64 Mn2 N21 O2 S4	C37.50 H34.50 Mn N10.50 O S2
Mr	1529.59	767.31
Dx,g cm-3	1.336	1.340
Z	2	4
Mu (mm-1)	0.502	0.502
F000	1582.0	1592.0
F000’	1584.76	
h,k,lmax	17,18,26	17,18,26
Nref	18442	17782
Tmin,Tmax	0.836,0.879	0.841,0.882
Tmin’	0.836	

Correction method= # Reported T Limits: Tmin=0.841 Tmax=0.882
AbsCorr = EMPIRICAL

Data completeness= 0.964 Theta(max)= 28.041

R(reflections)= 0.1035(10537) wR2(reflections)= 0.2566(17782)

S = 1.137 Npar= 942

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 A

PLAT430_ALERT_2_A Short Inter D...A Contact O2' ..O2' . 1.42 Ang.
1-x,2-y,1-z = 2_676 Check

Alert level C

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by .. 5.03 Check
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)... Please Check
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ..... 0.26 Report
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density .... 2.63 Report
PLAT220_ALERT_2_C Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 3.7 Ratio
PLAT222_ALERT_3_C Non-Solv. Resd 1 H Uiso(max)/Uiso(min) Range 4.6 Ratio
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of S1 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of S2 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C11 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C17 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of S1A Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of S2A Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C7 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of N11 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including O1 0.202 Check
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.00836 Ang.
PLAT420_ALERT_2_C D-H Without Acceptor N10A --H10P . Please Check
PLAT601_ALERT_2_C Structure Contains Solvent Accessible VOIDS of . 87 Ang**3

Alert level G

FORMU01_ALERT_1_G There is a discrepancy between the atom counts in the
_chemical_formula_sum and _chemical_formula_moiety. This is
usually due to the moiety formula being in the wrong format.
Atom count from _chemical_formula_sum: C37.5 H34.5 Mn1 N10.5 O1 S2
Atom count from _chemical_formula_moiety:C37.5 H34.5 N11.5 O1.5 S2
FORMU01_ALERT_2_G There is a discrepancy between the atom counts in the
_chemical_formula_sum and the formula from the _atom_site* data.
Atom count from _chemical_formula_sum:C37.5 H34.5 Mn1 N10.5 O1 S2
Atom count from the _atom_site data: C37.5 H32 Mn1 N10.5 O1 S2
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G WARNING: H atoms missing from atom site list. Is this intentional?
From the CIF: _cell_formula_units_Z 4
From the CIF: _chemical_formula_sum C37.50 H34.50 Mn N10.50 O S2
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	150.00	150.00	0.00
H	138.00	128.00	10.00
Mn	4.00	4.00	0.00
N	42.00	42.00	0.00
O	4.00	4.00	0.00
S	8.00	8.00	0.00

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 4 Report
PLAT012_ALERT_1_G N.O.K. _shelx_res_checksum Found in CIF ..... Please Check
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.50 Check
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.10 Report

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PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          1 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)        293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)        293 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O2         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O2'        Constrained at        0.5 Check
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
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... Resd  4           0.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... Resd  5           0.50 Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....         O2 Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....        O2' Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  O2       ..C37              2.90 Ang.
                                                 x,-1+y,z  =      1_545 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Mn1       (II)      .        2.19 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Mn1A      (II)      .        2.17 Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
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1 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
19 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
25 **ALERT level G** = General information/check it is not something unexpected

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

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checkCIF publication errors

Alert level A

```
PUBL004_ALERT_1_A  The contact author's name and address are missing,
           _publ_contact_author_name and _publ_contact_author_address.
PUBL005_ALERT_1_A  _publ_contact_author_email, _publ_contact_author_fax and
           _publ_contact_author_phone are all missing.
           At least one of these should be present.
PUBL006_ALERT_1_A  _publ_requested_journal is missing
           e.g. 'Acta Crystallographica Section C'
PUBL008_ALERT_1_A  _publ_section_title is missing. Title of paper.
PUBL009_ALERT_1_A  _publ_author_name is missing. List of author(s) name(s).
PUBL010_ALERT_1_A  _publ_author_address is missing. Author(s) address(es).
PUBL012_ALERT_1_A  _publ_section_abstract is missing.
           Abstract of paper in English.
```

Alert level G

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PUBL017_ALERT_1_G The _publ_section_references section is missing or
           empty.
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7 **ALERT level A** = Data missing that is essential or data in wrong format
1 **ALERT level G** = General alerts. Data that may be required is missing

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Publication of your CIF

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.

If level A alerts remain, which you believe to be justified deviations, and you intend to submit this CIF for publication in a journal, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. This will allow your explanation to be considered as part of the review process.

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_PUBL004_GLOBAL
;
PROBLEM: The contact author’s name and address are missing,
RESPONSE: ...
;
_vrf_PUBL005_GLOBAL
;
PROBLEM: _publ_contact_author_email, _publ_contact_author_fax and
RESPONSE: ...
;
_vrf_PUBL006_GLOBAL
;
PROBLEM: _publ_requested_journal is missing
RESPONSE: ...
;
_vrf_PUBL008_GLOBAL
;
PROBLEM: _publ_section_title is missing. Title of paper.
RESPONSE: ...
;
_vrf_PUBL009_GLOBAL
;
PROBLEM: _publ_author_name is missing. List of author(s) name(s).
RESPONSE: ...
;
_vrf_PUBL010_GLOBAL
;
PROBLEM: _publ_author_address is missing. Author(s) address(es).
RESPONSE: ...
;
_vrf_PUBL012_GLOBAL
;
PROBLEM: _publ_section_abstract is missing.
```

```
RESPONSE: ...
;
_vrf_PLAT430_I
;
PROBLEM: Short Inter D...A Contact  O2'      ..O2'      .       1.42 Ang.
RESPONSE: ...
;
# end Validation Reply Form
```

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If you wish to submit your CIF for publication in IUCrData you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

PLATON version of 07/08/2019; check.def file version of 30/07/2019

Datablock I - ellipsoid plot