

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) I

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 = 0.0052 Å Wavelength=0.71073

Cell: a=10.4921(4) b=10.5763(4) c=12.4197(5)
 alpha=70.893(2) beta=66.685(2) gamma=82.624(2)

Temperature: 293 K

	Calculated	Reported
Volume	1195.92(8)	1195.92(8)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C22 H20 F6 Mn O6	C22 H20 F6 Mn O6
Sum formula	C22 H20 F6 Mn O6	C22 H20 F6 Mn O6
Mr	549.32	549.32
Dx,g cm-3	1.526	1.525
Z	2	2
Mu (mm-1)	0.634	0.634
F000	558.0	558.0
F000'	559.09	
h,k,lmax	13,13,16	13,13,16
Nref	5578	5457
Tmin,Tmax	0.927,0.981	0.858,0.981
Tmin'	0.853	

Correction method= # Reported T Limits: Tmin=0.858 Tmax=0.981
AbsCorr = MULTI-SCAN

Data completeness= 0.978 Theta(max)= 27.632

R(reflections)= 0.0459(3656) wR2(reflections)= 0.1264(5457)

S = 1.011 Npar= 353

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

PLAT213_ALERT_2_C	Atom F5B	has ADP max/min Ratio	3.1	prolat
PLAT241_ALERT_2_C	High 'MainMol'	Ueq as Compared to Neighbors of	C9	Check
PLAT910_ALERT_3_C	Missing # of FCF	Reflection(s) Below Theta(Min).	9	Note
PLAT911_ALERT_3_C	Missing FCF Refl	Between Thmin & STh/L= 0.600	24	Report



Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle	Restraints on AtSite	4	Note
PLAT066_ALERT_1_G	Predicted and Reported Tmin&	Tmax Range Identical	?	Check
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles	are Equal ..(Note)	0.002	Degree
PLAT172_ALERT_4_G	The CIF-Embedded .res File	Contains DFIX Records	1	Report
PLAT199_ALERT_1_G	Reported _cell_measurement_	temperature	293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_	temperature	293	Check
PLAT242_ALERT_2_G	Low 'MainMol'	Ueq as Compared to Neighbors of	C1	Check
PLAT242_ALERT_2_G	Low 'MainMol'	Ueq as Compared to Neighbors of	C11	Check
PLAT301_ALERT_3_G	Main Residue Disorder	(Resd 1)	9%	Note
PLAT434_ALERT_2_G	Short Inter HL..HL Contact	F1 ..F1	2.81	Ang.
		1-x,1-y,1-z =	2_666	Check
PLAT794_ALERT_5_G	Tentative Bond Valency for Mn1	(II)	2.21	Info
PLAT860_ALERT_3_G	Number of Least-Squares	Restraints	2	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections	Above STh/L= 0.600	87	Note
PLAT913_ALERT_3_G	Missing # of Very Strong	Reflections in FCF	1	Note
PLAT933_ALERT_2_G	Number of OMIT Records in	Embedded .res File ...	1	Note
PLAT941_ALERT_3_G	Average HKL Measurement	Multiplicity	1.7	Low
PLAT978_ALERT_2_G	Number C-C Bonds with	Positive Residual Density.	3	Info
PLAT992_ALERT_5_G	Repd & Actual _reflns_	number_gt Values Differ by	2	Check

-
- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
 0 **ALERT level B** = A potentially serious problem, consider carefully
 4 **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
- 4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 8 ALERT type 2 Indicator that the structure model may be wrong or deficient
 6 ALERT type 3 Indicator that the structure quality may be low
 2 ALERT type 4 Improvement, methodology, query or suggestion
 2 ALERT type 5 Informative message, check
-

checkCIF publication errors



Alert level A

PUBL012_ALERT_1_A _publ_section_abstract is missing.
 Abstract of paper in English.



Alert level G

PUBL017_ALERT_1_G The _publ_section_references section is missing or empty.

-
- 1 **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
-

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_PUBL012_GLOBAL
;
PROBLEM: _publ_section_abstract is missing.
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.

