

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 = 0.0035 Å Wavelength=0.71073

Cell: a=16.1805(3) b=10.5318(2) c=17.8217(3)
 alpha=90 beta=91.558(2) gamma=90

Temperature: 293 K

	Calculated	Reported
Volume	3035.87(10)	3035.87(10)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C30 H22 F6 Mn N2 O6	C30 H22 F6 Mn N2 O6
Sum formula	C30 H22 F6 Mn N2 O6	C30 H22 F6 Mn N2 O6
Mr	675.44	675.43
Dx,g cm-3	1.478	1.478
Z	4	4
Mu (mm-1)	0.517	0.517
F000	1372.0	1372.0
F000'	1374.26	
h,k,lmax	21,13,23	21,13,23
Nref	6956	6949
Tmin,Tmax	0.883,0.950	0.703,1.000
Tmin'	0.772	

Correction method= # Reported T Limits: Tmin=0.703 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.999 Theta(max)= 27.482

R(reflections)= 0.0416(4910) wR2(reflections)= 0.1162(6949)

S = 1.051 Npar= 471

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

PLAT112_ALERT_2_B ADDSYM Detects New (Pseudo) Symm. Elem C 97 %Fit

Author Response: Possible pseudo-translation was detected, however, no additional space group can be found using the Platon program.



Alert level C

PLAT213_ALERT_2_C Atom F2B	has ADP max/min Ratio	3.4	prolat
PLAT213_ALERT_2_C Atom F3B	has ADP max/min Ratio	3.2	prolat
PLAT213_ALERT_2_C Atom F5B	has ADP max/min Ratio	3.2	prolat
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of		C25	Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of		C19	Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of		N1	Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of		C23	Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor		2.1	Note
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance		4.701	Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min).		8	Note
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..		1	Check



Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite		4	Note
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
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)	13%	Note
PLAT301_ALERT_3_G Main Residue Disorder	(Resd 2)	13%	Note
PLAT794_ALERT_5_G Tentative Bond Valency for Mn1	(II)	2.20	Info
PLAT794_ALERT_5_G Tentative Bond Valency for Mn2	(II)	2.23	Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints		2	Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity		4.2	Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.		5	Info

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

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

Datablock I - ellipsoid plot

