

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 = 0.0041 A	Wavelength=1.54178
Cell:	a=13.1706(1)	b=18.5816(2) c=51.0054(5)
	alpha=90	beta=92.016(1) gamma=90
Temperature:	123 K	
	Calculated	Reported
Volume	12474.9(2)	12474.9(2)
Space group	C 2/c	C 2/c
Hall group	-C 2yc	-C 2yc
Moiety formula	2(C36 Al F46 O3), 2(C10 H10 Mo2 P6), 3(C H2 Cl2)	2(C36 Al F46 O3), 2(C10 H10 Mo2 P6), 3(C H2 Cl2)
Sum formula	C95 H26 Al2 Cl6 F92 Mo4 O6 P12	C95 H26 Al2 Cl6 F92 Mo4 O6 P12
Mr	4033.22	4033.22
Dx, g cm-3	2.148	2.148
Z	4	4
Mu (mm-1)	7.793	7.779
F000	7792.0	7792.0
F000'	7850.04	
h,k,lmax	15,21,60	15,21,60
Nref	10845	10672
Tmin,Tmax	0.098,0.147	0.165,0.338
Tmin'	0.027	

Correction method= ANALYTICAL

Data completeness= 0.984 Theta(max)= 65.820

R(reflections)= 0.0325(9496) wR2(reflections)= 0.0896(10672)

S = 1.033 Npar= 1091

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

PLAT088_ALERT_3_C	Poor Data / Parameter Ratio	9.94
PLAT213_ALERT_2_C	Atom C44 has ADP max/min Ratio	3.2 oblate
PLAT220_ALERT_2_C	Large Non-Solvent C Ueq(max)/Ueq(min) ...	3.4 Ratio



Alert level G

PLAT143_ALERT_4_G	su on c - Axis Small or Missing	0.00050 Ang.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Mo1 -- P1 ..	9.8 su
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Mo1 -- P2 ..	8.8 su
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Mo1 -- P3 ..	9.3 su
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Mo1 -- P1_a ..	9.3 su
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Mo1 -- P2_a ..	9.0 su
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Mo1 -- P3_a ..	9.5 su
PLAT301_ALERT_3_G	Main Residue Disorder	Percentage = 13 Note
PLAT302_ALERT_4_G	Anion/Solvent Disorder	Percentage = 100 Note
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F6 .. F15 .	2.81 Ang.
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F8 .. F29 .	2.83 Ang.
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F24 .. F46 .	2.73 Ang.
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F28 .. F37 .	2.71 Ang.
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F30 .. F36 .	2.64 Ang.
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F35 .. F44 .	2.82 Ang.
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	73 Note

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
3 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
16 **ALERT level G** = General information/check it is not something unexpected
- 0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
14 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
2 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

checkCIF publication errors



Alert level A

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.

- 1 **ALERT level A** = Data missing that is essential or data in wrong format
0 **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.

```
# start Validation Reply Form
_vrf_PUBL005_GLOBAL
;
PROBLEM: _publ_contact_author_email, _publ_contact_author_fax and
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 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 18/09/2013; check.def file version of 12/09/2013

