

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) d\_sc\_005\_final

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: d\_sc\_005\_final

---

Bond precision:	C-C = 0.0094 A	Wavelength=1.54178
Cell:	a=15.1833 (6)	b=13.4972 (4)      c=24.4882 (9)
	alpha=90	beta=90      gamma=90
Temperature:	100 K	
	Calculated	Reported
Volume	5018.4 (3)	5018.4 (3)
Space group	P b c a	P b c a
Hall group	-P 2ac 2ab	-P 2ac 2ab
Moiety formula	C21 H18 F6 Mn N6 O7 S2	C21 H18 F6 Mn N6 O7 S2
Sum formula	C21 H18 F6 Mn N6 O7 S2	C21 H18 F6 Mn N6 O7 S2
Mr	699.47	699.47
Dx, g cm <sup>-3</sup>	1.852	1.852
Z	8	8
Mu (mm <sup>-1</sup> )	6.790	6.790
F000	2824.0	2824.0
F000'	2835.59	
h, k, lmax	18, 16, 29	18, 16, 29
Nref	4598	4579
Tmin, Tmax	0.409, 0.504	0.243, 0.547
Tmin'	0.121	

Correction method= # Reported T Limits: Tmin=0.243 Tmax=0.547  
AbsCorr = MULTI-SCAN

Data completeness= 0.996      Theta(max)= 68.238

R(reflections)= 0.0816 ( 3561)	wR2(reflections)= 0.1905 ( 4579)
S = 1.177	Npar= 394

---

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

RINTA01\_ALERT\_3\_C The value of Rint is greater than 0.12  
Rint given 0.170

PLAT020_ALERT_3_C	The Value of Rint is Greater Than 0.12 .....	0.170	Report
PLAT213_ALERT_2_C	Atom N6 has ADP max/min Ratio .....	3.1	oblate
PLAT213_ALERT_2_C	Atom C15 has ADP max/min Ratio .....	3.8	oblate
PLAT341_ALERT_3_C	Low Bond Precision on C-C Bonds .....	0.00936	Ang.
PLAT790_ALERT_4_C	Centre of Gravity not Within Unit Cell: Resd. #	1	Note
	C21 H18 F6 Mn N6 O7 S2		
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance .....	7.774	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance .....	2.109	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & Sth/L= 0.600	19	Report
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 1.01Ang From O22	0.42	eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 0.83Ang From O21	0.42	eA-3

---

### Alert level G

PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	17	Report
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	33.95	Why ?
PLAT177_ALERT_4_G	The CIF-Embedded .res File Contains DELU Records	1	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	1	Report
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used	0.0050	Report
PLAT192_ALERT_3_G	A Non-default DELU Restraint Value for First Par	0.0050	Report
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F13 ..F13	2.80	Ang.
	-x,1-y,-1-z =	5_564	Check
PLAT794_ALERT_5_G	Tentative Bond Valency for Mn1 (II)	1.95	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....	110	Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary		Please Do !
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	1	Note
PLAT965_ALERT_2_G	The SHELXL WEIGHT Optimisation has not Converged		Please Check
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	3	Info

---

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

## 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**

PUBL017\_ALERT\_1\_G The \_publ\_section\_references section is missing or  
empty.

---

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

---

## **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_RINTA01_d_sc_005_final
;
PROBLEM: The value of Rint is greater than 0.12
RESPONSE: ...
;
_vrf_PLAT020_d_sc_005_final
;
PROBLEM: The Value of Rint is Greater Than 0.12 ..... 0.170 Report
RESPONSE: ...
;
_vrf_PLAT213_d_sc_005_final
;
PROBLEM: Atom N6                has ADP max/min Ratio ..... 3.1 oblate
RESPONSE: ...
;
_vrf_PLAT341_d_sc_005_final
;
PROBLEM: Low Bond Precision on  C-C Bonds ..... 0.00936 Ang.
RESPONSE: ...
;
_vrf_PLAT790_d_sc_005_final

```

```

;
PROBLEM: Centre of Gravity not Within Unit Cell: Resd. #          1 Note
RESPONSE: ...
;
_vrf_PLAT906_d_sc_005_final
;
PROBLEM: Large K Value in the Analysis of Variance ..... 7.774 Check
RESPONSE: ...
;
_vrf_PLAT911_d_sc_005_final
;
PROBLEM: Missing FCF Refl Between Thmin & STh/L=      0.600      19 Report
RESPONSE: ...
;
_vrf_PLAT975_d_sc_005_final
;
PROBLEM: Check Calcd Resid. Dens.  1.01Ang From O22      .      0.42 eA-3
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 06/07/2023; check.def file version of 30/06/2023**

