

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 = 0.0079 A Wavelength=0.71073

Cell: a=9.5600(19) b=11.746(2) c=12.911(3)
alpha=87.45(3) beta=70.06(3) gamma=79.44(3)

Temperature: 200 K

	Calculated	Reported
Volume	1339.6(6)	1339.6(6)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C62 H44 Br4 Mg N8 O2	?
Sum formula	C62 H44 Br4 Mg N8 O2	C62 H44 Br4 Mg N8 O2
Mr	1276.96	1277.00
Dx, g cm ⁻³	1.583	1.583
Z	1	1
Mu (mm ⁻¹)	3.070	3.070
F000	640.0	640.0
F000'	639.10	
h, k, lmax	11, 14, 15	11, 14, 15
Nref	5266	5095
Tmin, Tmax	0.483, 0.692	0.378, 1.000
Tmin'	0.290	

Correction method= # Reported T Limits: Tmin=0.378 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.968 Theta(max)= 25.999

R(reflections)= 0.0578(4025) wR2(reflections)=
0.1585(5095)

S = 1.123 Npar= 349

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**

PLAT196_ALERT_1_B No TEMP record and _measurement_temperature .NE. 293 Degree

 **Alert level C**

PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.8 Ratio
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C25 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C24 Check
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds 0.00794 Ang.
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 47 Report

 **Alert level G**

PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.03 Degree
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). 2 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 122 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ... 1 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 2 Note
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res .. 52.0 Degree
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 1 Info

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

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

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_PLAT196_I
;
PROBLEM: No TEMP record and _measurement_temperature .NE. 293 Degree
RESPONSE: ...
;
_vrf_PLAT220_I
;
PROBLEM: NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.8 Ratio
RESPONSE: ...
;
```

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_vrf_PLAT241_I
;
PROBLEM: High 'MainMol' Ueq as Compared to Neighbors of C25 Check
RESPONSE: ...
;
_vrf_PLAT242_I
;
PROBLEM: Low 'MainMol' Ueq as Compared to Neighbors of C24 Check
RESPONSE: ...
;
_vrf_PLAT341_I
;
PROBLEM: Low Bond Precision on C-C Bonds ..... 0.00794 Ang.
RESPONSE: ...
;
_vrf_PLAT911_I
;
PROBLEM: Missing FCF Refl Between Thmin & STh/L= 0.600 47 Report
RESPONSE: ...
;
# end Validation Reply Form

```

It is advisable to 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 purpose of your study may justify the reported deviations and the more serious of these should normally 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.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

