

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) aaa

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: aaa

Bond precision: C-C = 0.0117 Å Wavelength=0.71073

Cell: a=13.267(2) b=16.259(3) c=22.397(3)
 alpha=74.897(6) beta=85.589(7) gamma=84.927(7)

Temperature: 296 K

	Calculated	Reported
Volume	4638.8(13)	4639.0(13)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	2(C54 H36 N4 O), C H Cl3 [+ solvent]	C H Cl3, 2(C54 H36 N4 O)
Sum formula	C109 H73 Cl3 N8 O2 [+ solvent]	C109 H73 Cl3 N8 O2
Mr	1633.10	1633.10
Dx, g cm ⁻³	1.169	1.169
Z	2	2
Mu (mm ⁻¹)	0.153	0.153
F000	1700.0	1700.0
F000'	1701.48	
h,k,lmax	15,19,26	15,19,26
Nref	16350	16104
Tmin,Tmax	0.970,0.977	0.507,0.746
Tmin'	0.970	

Correction method= # Reported T Limits: Tmin=0.507 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.985 Theta(max)= 25.000


R(reflections)= 0.1047(4523) wR2(reflections)= 0.2671(16104)

S = 0.920 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 A**

PLAT026_ALERT_3_A Ratio Observed / Unique Reflections (too) Low .. 28% Check

 **Alert level B**

PLAT340_ALERT_3_B Low Bond Precision on C-C Bonds 0.0117 Ang.

 **Alert level C**

RINTA01_ALERT_3_C The value of Rint is greater than 0.12

Rint given 0.122

PLAT020_ALERT_3_C The Value of Rint is Greater Than 0.12 0.122 Report

PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) 0.27 Report

PLAT230_ALERT_2_C Hirshfeld Test Diff for N3 --C103 . 5.4 s.u.

PLAT230_ALERT_2_C Hirshfeld Test Diff for C55 --C56 . 5.9 s.u.

PLAT230_ALERT_2_C Hirshfeld Test Diff for C81 --C82 . 6.2 s.u.

PLAT234_ALERT_4_C Large Hirshfeld Difference N7 --C40 . 0.17 Ang.

PLAT234_ALERT_4_C Large Hirshfeld Difference C4 --C12 . 0.16 Ang.

PLAT234_ALERT_4_C Large Hirshfeld Difference C14 --C15 . 0.17 Ang.

PLAT234_ALERT_4_C Large Hirshfeld Difference C15 --C18 . 0.17 Ang.

PLAT234_ALERT_4_C Large Hirshfeld Difference C22 --C23 . 0.16 Ang.

PLAT234_ALERT_4_C Large Hirshfeld Difference C26 --C27 . 0.19 Ang.

PLAT234_ALERT_4_C Large Hirshfeld Difference C28 --C29 . 0.20 Ang.

PLAT234_ALERT_4_C Large Hirshfeld Difference C37 --C42 . 0.16 Ang.

PLAT234_ALERT_4_C Large Hirshfeld Difference C44 --C45 . 0.18 Ang.

PLAT234_ALERT_4_C Large Hirshfeld Difference C45 --C46 . 0.21 Ang.

PLAT234_ALERT_4_C Large Hirshfeld Difference C50 --C51 . 0.16 Ang.

PLAT234_ALERT_4_C Large Hirshfeld Difference N3 --C94 . 0.21 Ang.

PLAT234_ALERT_4_C Large Hirshfeld Difference C56 --C57 . 0.18 Ang.

PLAT234_ALERT_4_C Large Hirshfeld Difference C57 --C58 . 0.20 Ang.

PLAT234_ALERT_4_C Large Hirshfeld Difference C61 --C62 . 0.16 Ang.

PLAT234_ALERT_4_C Large Hirshfeld Difference C71 --C91 . 0.16 Ang.

PLAT234_ALERT_4_C Large Hirshfeld Difference C82 --C83 . 0.18 Ang.

PLAT234_ALERT_4_C Large Hirshfeld Difference C92 --C93 . 0.21 Ang.

PLAT234_ALERT_4_C Large Hirshfeld Difference C95 --C96 . 0.18 Ang.

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C8 Check

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C69 Check

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C72 Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C25 Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C68 Check

PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C109 Check

PLAT260_ALERT_2_C Large Average Ueq of Residue Including C11 0.165 Check

PLAT331_ALERT_2_C Small Aver Phenyl C-C Dist C25 --C30 . 1.37 Ang.

PLAT331_ALERT_2_C Small Aver Phenyl C-C Dist C31 --C36 . 1.37 Ang.

PLAT331_ALERT_2_C Small Aver Phenyl C-C Dist C97 --C102 . 1.37 Ang.

PLAT369_ALERT_2_C Long C(sp2)-C(sp2) Bond C70 - C73 . 1.53 Ang.

PLAT411_ALERT_2_C Short Inter H...H Contact H107 ..H107 . 2.12 Ang.

-x,1-y,-z = 2_565 Check

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 15.910 Check

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 6.160 Check

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 3.367 Check

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 2.214 Check

PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min). 10 Note

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.595 237 Report

● Alert level G

PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	27	Report
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ		Please Check
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	2	Report
PLAT187_ALERT_4_G	The CIF-Embedded .res File Contains RIGU Records	3	Report
PLAT335_ALERT_2_G	Check Large C6 Ring C-C Range C13 -C16	0.15	Ang.
PLAT335_ALERT_2_G	Check Large C6 Ring C-C Range C67 -C72	0.17	Ang.
PLAT606_ALERT_4_G	Solvent Accessible VOID(S) in Structure		! Info
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. # C H C13	3	Note
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	171	Note
PLAT868_ALERT_4_G	ALERTS Due to the Use of _smtbx_masks Suppressed		! Info
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .		Please Do !
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	17	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	2.0	Low
PLAT961_ALERT_5_G	Dataset Contains no Negative Intensities		Please Check
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	0	Info

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- 1 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
43 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
15 **ALERT level G** = General information/check it is not something unexpected
- 2 **ALERT type 1** CIF construction/syntax error, inconsistent or missing data
19 **ALERT type 2** Indicator that the structure model may be wrong or deficient
13 **ALERT type 3** Indicator that the structure quality may be low
25 **ALERT type 4** Improvement, methodology, query or suggestion
1 **ALERT type 5** Informative message, check
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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.

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_RINTA01_aaa
;
PROBLEM: The value of Rint is greater than 0.12
RESPONSE: ...
;
_vrf_PLAT026_aaa
;
PROBLEM: Ratio Observed / Unique Reflections (too) Low ..          28% Check
RESPONSE: ...
;
_vrf_PLAT020_aaa
;
PROBLEM: The Value of Rint is Greater Than 0.12 .....          0.122 Report
RESPONSE: ...
;
_vrf_PLAT084_aaa
;
PROBLEM: High wR2 Value (i.e. > 0.25) .....          0.27 Report
RESPONSE: ...
;
_vrf_PLAT230_aaa
;
PROBLEM: Hirshfeld Test Diff for      N3      --C103      .          5.4 s.u.
RESPONSE: ...
;
_vrf_PLAT234_aaa
;
PROBLEM: Large Hirshfeld Difference N7      --C40      .          0.17 Ang.
RESPONSE: ...
;
_vrf_PLAT241_aaa
;
PROBLEM: High      'MainMol' Ueq as Compared to Neighbors of          C8 Check
RESPONSE: ...
;
_vrf_PLAT242_aaa
;
PROBLEM: Low      'MainMol' Ueq as Compared to Neighbors of          C25 Check
RESPONSE: ...
;
_vrf_PLAT244_aaa
;
PROBLEM: Low      'Solvent' Ueq as Compared to Neighbors of          C109 Check
RESPONSE: ...
;
_vrf_PLAT260_aaa
;
PROBLEM: Large Average Ueq of Residue Including          C11          0.165 Check
RESPONSE: ...
;
_vrf_PLAT331_aaa
;
PROBLEM: Small Aver Phenyl C-C Dist C25      --C30      .          1.37 Ang.
RESPONSE: ...
;
_vrf_PLAT369_aaa
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;
PROBLEM: Long C(sp2)-C(sp2) Bond C70 - C73 . 1.53 Ang.
RESPONSE: ...
;
_vrf_PLAT411_aaa
;
PROBLEM: Short Inter H...H Contact H107 ..H107 . 2.12 Ang.
RESPONSE: ...
;
_vrf_PLAT906_aaa
;
PROBLEM: Large K Value in the Analysis of Variance ..... 15.910 Check
RESPONSE: ...
;
_vrf_PLAT910_aaa
;
PROBLEM: Missing # of FCF Reflection(s) Below Theta(Min). 10 Note
RESPONSE: ...
;
_vrf_PLAT911_aaa
;
PROBLEM: Missing FCF Refl Between Thmin & STh/L= 0.595 237 Report
RESPONSE: ...
;
# end Validation Reply Form
```

PLATON version of 10/08/2020; check.def file version of 06/08/2020

