

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 = 0.0064 A	Wavelength=0.71073	
Cell:	a=14.1676(17)	b=16.033(2)	c=24.954(4)
	alpha=90	beta=93.491(5)	gamma=90
Temperature:	150 K		
	Calculated	Reported	
Volume	5657.8(13)	5657.9(14)	
Space group	P 21/n	P 21/n	
Hall group	-P 2yn	-P 2yn	
Moiety formula	C65 H47 N7 O6, C H Cl3, C H4 O	C65 H47 N7 O6, C H Cl3, C H4 O	
Sum formula	C67 H52 Cl3 N7 O7	C67 H52 Cl3 N7 O7	
Mr	1173.51	1173.50	
Dx, g cm ⁻³	1.378	1.378	
Z	4	4	
Mu (mm ⁻¹)	0.226	0.226	
F000	2440.0	2440.0	
F000'	2442.75		
h,k,lmax	18,20,32	18,20,32	
Nref	12825	12698	
Tmin,Tmax	0.929,0.967	0.627,0.967	
Tmin'	0.909		

Correction method= # Reported T Limits: Tmin=0.627 Tmax=0.967
AbsCorr = MULTI-SCAN

Data completeness= 0.990 Theta(max)= 27.365

R(reflections)= 0.1015(6599) wR2(reflections)= 0.3021(12698)

S = 1.031 Npar= 789

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

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75
The relevant atom site should be identified.

RINTA01_ALERT_3_C The value of Rint is greater than 0.12
Rint given 0.157

PLAT020_ALERT_3_C The Value of Rint is Greater Than 0.12 0.157 Report

PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) 0.30 Report

PLAT097_ALERT_2_C Large Reported Max. (Positive) Residual Density 1.46 eA-3

PLAT213_ALERT_2_C Atom C72 has ADP max/min Ratio 3.2 prolat

PLAT213_ALERT_2_C Atom C73 has ADP max/min Ratio 3.3 prolat

PLAT213_ALERT_2_C Atom C72B has ADP max/min Ratio 3.2 prolat

PLAT213_ALERT_2_C Atom C73B has ADP max/min Ratio 3.3 prolat

PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.4 Ratio

PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C101 Check

PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor 2.2 Note

PLAT260_ALERT_2_C Large Average Ueq of Residue Including C11 0.162 Check

PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds 0.00643 Ang.

PLAT414_ALERT_2_C Short Intra D-H..H-X H27N ..H35 1.93 Ang.
x,y,z = 1_555 Check

PLAT414_ALERT_2_C Short Intra D-H..H-X H57N ..H65 1.95 Ang.
x,y,z = 1_555 Check

PLAT420_ALERT_2_C D-H Without Acceptor N27 --H27N . Please Check

PLAT420_ALERT_2_C D-H Without Acceptor N57 --H57N . Please Check

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 7.738 Check

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 2.012 Check

PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta (Min). 5 Note

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 50 Report

PLAT975_ALERT_2_C Check Calcd Resid. Dens. 1.03A From O42 0.60 eA-3

PLAT977_ALERT_2_C Check Negative Difference Density on H410 -0.35 eA-3

● Alert level G

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 1 Report

PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.13 Report

PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 8.43 Why ?

PLAT168_ALERT_4_G The CIF-Embedded .res File Contains EXYZ Records 2 Report

PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 6 Report

PLAT301_ALERT_3_G Main Residue Disorder(Resd 1) 8% Note

PLAT335_ALERT_2_G Check Large C6 Ring C-C Range C71B -C76B 0.19 Ang.

PLAT412_ALERT_2_G Short Intra XH3 .. XHn H73 ..H78C . 2.14 Ang.
x,y,z = 1_555 Check

PLAT412_ALERT_2_G Short Intra XH3 .. XHn H78C ..H73B . 1.97 Ang.
x,y,z = 1_555 Check

PLAT432_ALERT_2_G Short Inter X...Y Contact C12 ..C75B 3.00 Ang.
3/2-x,-1/2+y,1/2-z = 2_645 Check

PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 74 Note

PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 3.7 Low

PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 2 Info

0 ALERT level A = Most likely a serious problem - resolve or explain

0 ALERT level B = A potentially serious problem, consider carefully

24 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

21 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
4 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: ...
;
# 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 05/12/2020; check.def file version of 05/12/2020

