

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 = 0.0063 A	Wavelength=1.54184
Cell:	a=25.014(2)	b=7.5767(5) c=44.880(4)
	alpha=90	beta=103.338(9) gamma=90
Temperature:	150 K	
	Calculated	Reported
Volume	8276.4(12)	8276.4(12)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	2(C60 H36), 1.5(C6 H6)	2(C60 H36), 1.5(C6 H6)
Sum formula	C129 H81	C129 H81
Mr	1630.94	1630.93
Dx,g cm-3	1.309	1.309
Z	4	4
Mu (mm-1)	0.563	0.563
F000	3420.0	3420.0
F000'	3428.91	
h,k,lmax	31,9,56	31,9,55
Nref	17352	16780
Tmin,Tmax	0.874,0.945	0.654,1.000
Tmin'	0.845	
Correction method=	# Reported T Limits: Tmin=0.654 Tmax=1.000	
AbsCorr =	MULTI-SCAN	
Data completeness=	0.967	Theta(max)= 76.200
R(reflections)=	0.0827(8676)	wR2(reflections)= 0.2624(16780)
S =	1.018	Npar= 1162

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

PLAT331_ALERT_2_B	Small Aver Phenyl C-C Dist	C1S	--C6S	.	1.35	Ang.
PLAT410_ALERT_2_B	Short Intra H...H Contact	H43A	..H47A	.	1.86	Ang.
			x,y,z	=	1_555	Check
PLAT410_ALERT_2_B	Short Intra H...H Contact	H23B	..H27B	.	1.89	Ang.
			x,y,z	=	1_555	Check

Alert level C

PLAT084_ALERT_3_C	High wR2 Value (i.e. > 0.25)	0.26	Report
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor	3.9	Note
PLAT340_ALERT_3_C	Low Bond Precision on C-C Bonds	0.00629	Ang.
PLAT410_ALERT_2_C	Short Intra H...H Contact	H3A ..H7A	.	1.96 Ang.
		x,y,z	=	1_555 Check
PLAT410_ALERT_2_C	Short Intra H...H Contact	H43B ..H47B	.	1.92 Ang.
		x,y,z	=	1_555 Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	11.038	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	2.375	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600	4	Report

Alert level G

PLAT908_ALERT_2_G	Max. Perc. Data with I > 2*s(I) per Res.Shell	.	74.40%	Note
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	554	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File	...	5	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	2.1	Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		0	Info

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

0 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
7 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

checkCIF publication errors

Alert level A

PUBL006_ALERT_1_A _publ_requested_journal is missing
e.g. 'Acta Crystallographica Section C'
PUBL009_ALERT_1_A _publ_author_name is missing. List of author(s) name(s).
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.

3 **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_PUBL006_GLOBAL
;
PROBLEM: _publ_requested_journal is missing
RESPONSE: ...
;
_vrf_PUBL009_GLOBAL
;
PROBLEM: _publ_author_name is missing. List of author(s) name(s).
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.

