

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 = 0.0048 Å Wavelength=0.71073

Cell: a=13.462(2) b=14.764(2) c=21.115(3)
 alpha=93.891(6) beta=99.656(5) gamma=94.702(6)

Temperature: 150 K

	Calculated	Reported
Volume	4109.0(10)	4108.9(10)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C65 H44 N7 O6 Pb [+ solvent]	C65 H44 N7 O6 Pb
Sum formula	C65 H44 N7 O6 Pb [+ solvent]	C65 H44 N7 O6 Pb
Mr	1226.28	1226.26
Dx, g cm ⁻³	0.991	0.991
Z	2	2
Mu (mm ⁻¹)	2.093	2.093
F000	1226.0	1226.0
F000'	1219.73	
h,k,lmax	17,19,27	17,19,27
Nref	18989	18330
Tmin,Tmax	0.729,0.794	0.673,0.794
Tmin'	0.551	

Correction method= # Reported T Limits: Tmin=0.673 Tmax=0.794
AbsCorr = MULTI-SCAN

Data completeness= 0.965 Theta(max)= 27.564

R(reflections)= 0.0383(16483) wR2(reflections)= 0.0923(18330)

S = 1.111 Npar= 516

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

PLAT029_ALERT_3_C	_diffrn_measured_fraction_theta_full	value	Low	.	0.970	Why?		
PLAT220_ALERT_2_C	NonSolvent	Resd	1	C	Ueq(max)/Ueq(min)	Range	3.6	Ratio
PLAT220_ALERT_2_C	NonSolvent	Resd	1	N	Ueq(max)/Ueq(min)	Range	4.8	Ratio
PLAT414_ALERT_2_C	Short Intra D-H..H-X	H47	..H55				1.94	Ang.
					x,y,z =		1_555	Check
PLAT420_ALERT_2_C	D-H Without Acceptor	N27	--H27	.				Please Check
PLAT420_ALERT_2_C	D-H Without Acceptor	N47	--H47	.				Please 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=	0.600				435	Report
PLAT934_ALERT_3_C	Number of (Iobs-Icalc)/Sigma(W)	> 10	Outliers	..			1	Check
PLAT977_ALERT_2_C	Check Negative Difference Density	on	H5				-0.40	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density	on	H76				-0.33	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density	on	H82				-0.35	eA-3

Alert level G

PLAT083_ALERT_2_G	SHELXL	Second	Parameter	in	WGHT	Unusually	Large	15.52	Why ?	
PLAT171_ALERT_4_G	The	CIF-Embedded	.res	File	Contains	EADP	Records	3	Report	
PLAT606_ALERT_4_G	Solvent	Accessible	VOID(S)	in	Structure		!	Info	
PLAT793_ALERT_4_G	Model	has	Chirality	at	C61	(Centro	SPGR)		S	Verify
PLAT794_ALERT_5_G	Tentative	Bond	Valency	for	Pb1	(II)	.	2.41	Info	
PLAT869_ALERT_4_G	ALERTS	Related	to	the	Use	of	SQUEEZE	Suppressed	!	Info
PLAT912_ALERT_4_G	Missing # of FCF Reflections	Above	STh/L=	0.600			213	Note		
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections	in	FCF			3	Note		
PLAT933_ALERT_2_G	Number of OMIT Records	in	Embedded	.res	File	...	4	Note		
PLAT941_ALERT_3_G	Average	HKL	Measurement	Multiplicity		3.9	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
0 **ALERT level B** = A potentially serious problem, consider carefully
12 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
11 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
11 ALERT type 2 Indicator that the structure model may be wrong or deficient
6 ALERT type 3 Indicator that the structure quality may be low
5 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.

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.

5 **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_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

Datablock I - ellipsoid plot

