

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) WHY1809

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: WHY1809

Bond precision: C-C = 0.0038 A Wavelength=0.71073

Cell: a=14.203(4) b=18.353(5) c=20.347(6)
 alpha=90 beta=93.656(8) gamma=90

Temperature: 296 K

	Calculated	Reported
Volume	5293(3)	5293(3)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C57 H35 Cl6 Eu N2 O6	C57 H35 Cl6 Eu N2 O6
Sum formula	C57 H35 Cl6 Eu N2 O6	C57 H35 Cl6 Eu N2 O6
Mr	1208.54	1208.53
Dx,g cm-3	1.517	1.517
Z	4	4
Mu (mm-1)	1.540	1.540
F000	2416.0	2416.0
F000'	2419.72	
h,k,lmax	18,24,26	18,23,26
Nref	12634	12234
Tmin,Tmax	0.656,0.735	0.672,0.748
Tmin'	0.643	

Correction method= # Reported T Limits: Tmin=0.672 Tmax=0.748
AbsCorr = MULTI-SCAN

Data completeness= 0.968 Theta(max)= 27.870

R(reflections)= 0.0258(10214) wR2(reflections)= 0.0628(12234)

S = 1.029 Npar= 650

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	Low	.	0.969	Why?
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	C6	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	C12	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	C14	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C4	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C7	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C10	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C13	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C22	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C37	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C43	Check
PLAT334_ALERT_2_C	Small Aver. Benzene C-C Dist	C4	-C9	1.37	Ang.
PLAT334_ALERT_2_C	Small Aver. Benzene C-C Dist	C10	-C15	1.37	Ang.
PLAT910_ALERT_3_C	Missing # of FCF Reflection(s) Below Theta(Min).			9	Note
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600		30	Report
PLAT913_ALERT_3_C	Missing # of Very Strong Reflections in FCF			16	Note

● Alert level G

PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF				Please Do !
PLAT794_ALERT_5_G	Tentative Bond Valency for Eul	(III)	.	2.92	Info
PLAT899_ALERT_4_G	SHELXL97 is Deprecated and Succeeded by SHELXL			2018	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600		340	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.			4	Info

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

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
13 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
2 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check

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.

PLATON version of 23/04/2018; check.def file version of 23/04/2018

