

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: p160621f

Bond precision: C-C = 0.0120 A

Wavelength=0.71073

Cell: a=11.6961(6) b=12.5891(6) c=19.3863(12)
 alpha=90.618(5) beta=104.979(5) gamma=95.282(4)
Temperature: 139 K

	Calculated	Reported
Volume	2744.0(3)	2744.0(3)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C43 H37 Eu F18 N4 O14	C43 H37 Eu F18 N4 O14
Sum formula	C43 H37 Eu F18 N4 O14	C43 H37 Eu F18 N4 O14
Mr	1327.74	1327.73
Dx,g cm-3	1.607	1.607
Z	2	2
Mu (mm-1)	1.267	1.267
F000	1320.0	1320.0
F000'	1320.74	
h,k,lmax	13,14,23	13,14,23
Nref	9660	9409
Tmin,Tmax		0.693,1.000
Tmin'		

Correction method= # Reported T Limits: Tmin=0.693 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.974

Theta(max)= 25.010

R(reflections)= 0.0808(7543)

wR2(reflections)= 0.2084(9409)

S = 1.099

Npar= 729

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	_diffn_measured_fraction_theta_full value Low .	0.974	Note
PLAT053_ALERT_1_C	Minimum Crystal Dimension Missing (or Error) ...		Please Check
PLAT054_ALERT_1_C	Medium Crystal Dimension Missing (or Error) ...		Please Check
PLAT055_ALERT_1_C	Maximum Crystal Dimension Missing (or Error) ...		Please Check
PLAT234_ALERT_4_C	Large Hirshfeld Difference F15 -- C39 ..	0.25	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C4 -- C5 ..	0.20	Ang.
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C12	Check
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds	0.012	Ang.
PLAT431_ALERT_2_C	Short Inter HL..A Contact F4 .. O2 ..	2.75	Ang.

● Alert level G

PLAT005_ALERT_5_G	No Embedded Refinement Details found in the CIF		Please Do !
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C29	Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C33	Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C34	Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C38	Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C39	Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C43	Check
PLAT605_ALERT_4_G	Largest Solvent Accessible VOID in Structure ...	269	A**3
PLAT869_ALERT_4_G	ALERTS Related to the use of SQUEEZE Suppressed		! Info

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

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
8 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 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

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.

