

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) HDS161202\_0m

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: HDS161202\_0m

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Bond precision:    C-C = 0.0093 A                      Wavelength=0.71073

Cell:                      a=12.0336(16)              b=21.134(3)              c=19.0963(17)  
                                    alpha=90                      beta=110.757(6)              gamma=90

Temperature:              296 K

	Calculated	Reported
Volume	4541.3(10)	4541.3(10)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C46 H32 Eu F9 N2 O6, 0.5(C6 H14)	C46 H32 Eu F9 N2 O6, 0.5(C6H14)
Sum formula	C49 H39 Eu F9 N2 O6	C49 H39 Eu F9 N2 O6
Mr	1074.79	1074.78
Dx,g cm-3	1.572	1.572
Z	4	4
Mu (mm-1)	1.470	1.470
F000	2156.0	2156.0
F000'	2156.64	
h,k,lmax	15,28,25	15,28,24
Nref	11141	11028
Tmin,Tmax	0.669,0.768	0.960,1.000
Tmin'	0.656	

Correction method= # Reported T Limits: Tmin=0.960 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.990                      Theta(max)= 28.164

R(reflections)= 0.0430( 7033)              wR2(reflections)= 0.1134( 11028)

S = 1.066                      Npar= 605

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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.

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**Alert level C**

PLAT230_ALERT_2_C	Hirshfeld Test Diff for	F6	--	C24	..	6.5 s.u.
PLAT230_ALERT_2_C	Hirshfeld Test Diff for	C25	--	C30	..	5.2 s.u.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C3	--	C4	..	0.16 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C5	--	C10	..	0.16 Ang.
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of					C10 Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of					C27 Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of					C34 Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of					C2S Check
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds .....					0.00927 Ang.
PLAT360_ALERT_2_C	Short C(sp3)-C(sp3) Bond	C2S	-	C3S	..	1.41 Ang.
PLAT905_ALERT_3_C	Negative K value in the Analysis of Variance ...					-1.140 Report
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				28 Report

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**Alert level G**

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite					5 Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...					4 Report
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ					Please Check
PLAT128_ALERT_4_G	Alternate Setting for Input Space Group	P21/c				P21/n Note
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records					3 Report
PLAT177_ALERT_4_G	The CIF-Embedded .res File Contains DELU Records					2 Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records					1 Report
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of					C12 Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of					C24 Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of					C36 Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels .....					7 Note
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....					11 Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600				66 Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...					3 Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.					1 Note

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

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

13 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

15 **ALERT level G** = General information/check it is not something unexpected

1 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

5 ALERT type 3 Indicator that the structure quality may be low

9 ALERT type 4 Improvement, methodology, query or suggestion

0 ALERT type 5 Informative message, check

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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.

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**PLATON version of 27/03/2017; check.def file version of 24/03/2017**

