

## 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: mo\_d8v3291\_0m\_morten

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Bond precision:    C-C = 0.0140 A                      Wavelength=0.71073

Cell:                      a=12.3655(14)              b=16.209(2)              c=20.711(3)  
                                    alpha=90                      beta=90                      gamma=90

Temperature:              122 K

	Calculated	Reported
Volume	4151.2(9)	4151.2(9)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C30 H24 F18 Fe La O12	C30 H24 F18 Fe La O12
Sum formula	C30 H24 F18 Fe La O12	C30 H24 F18 Fe La O12
Mr	1113.25	1113.25
Dx,g cm-3	1.781	1.781
Z	4	4
Mu (mm-1)	1.500	1.500
F000	2180.0	2180.0
F000'	2182.14	
h,k,lmax	16,21,27	16,21,27
Nref	10736[ 5917]	10728
Tmin,Tmax	0.537,0.651	0.539,0.746
Tmin'	0.320	

Correction method= # Reported T Limits: Tmin=0.539 Tmax=0.746  
AbsCorr = MULTI-SCAN

Data completeness= 1.81/1.00                      Theta(max)= 28.700

R(reflections)= 0.0543( 9561)                      wR2(reflections)= 0.1431( 10728)

S = 1.077    Npar= 584

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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**

PLAT213_ALERT_2_C	Atom F19	has ADP max/min Ratio .....	3.5	prolat
PLAT215_ALERT_3_C	Disordered F5#	has ADP max/min Ratio .....	3.6	Note
PLAT215_ALERT_3_C	Disordered F6#	has ADP max/min Ratio .....	3.1	Note
PLAT220_ALERT_2_C	Non-Solvent Resd 1 C	Ueq(max)/Ueq(min) Range	3.5	Ratio
PLAT234_ALERT_4_C	Large Hirshfeld Difference F2AA	--C7AA	0.23	Ang.
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of		C5AA	Check
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds .....		0.01404	Ang.

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● **Alert level G**

PLAT012_ALERT_1_G	No	_shelx_res_checksum Found in CIF .....		Please Check
PLAT063_ALERT_4_G	Crystal Size Likely too Large for Beam Size ....		0.75	mm
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large		18.76	Why ?
PLAT230_ALERT_2_G	Hirshfeld Test Diff for F15A	--F20	9.5	s.u.
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of		C1AA	Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of		C3AA	Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of		C9AA	Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of		C7AA	Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of		C18	Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of		C20	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of F4AA	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of F4AB	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of F15	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of F15A	Constrained at	0.5	Check
PLAT301_ALERT_3_G	Main Residue Disorder .....	(Resd 1 )	3%	Note
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond C7AA	- C16	1.53	Ang.
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels .....		25	Note
PLAT794_ALERT_5_G	Tentative Bond Valency for La1	(III)	3.47	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Fe2	(III)	3.11	Info
PLAT850_ALERT_4_G	Check Flack Parameter Exact Value 0.00 and s.u.		0.03	Check
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...		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  
7 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
21 **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  
4 ALERT type 3 Indicator that the structure quality may be low  
8 ALERT type 4 Improvement, methodology, query or suggestion  
2 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 23/04/2018; check.def file version of 23/04/2018**

