

# 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: shelx

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Bond precision:    C-C = 0.0084 A                      Wavelength=0.71073

Cell:                      a=28.1295(5)              b=15.2305(3)              c=8.7607(1)  
                                    alpha=90                      beta=98.835(1)              gamma=90

Temperature:              293 K

	Calculated	Reported
Volume	3708.78(11)	3708.78(11)
Space group	C 2/c	C 2/c
Hall group	-C 2yc	-C 2yc
Moiety formula	C15 H12 La O8, 2(O)	?
Sum formula	C15 H12 La O10	C15 H20 La O10
Mr	491.16	499.22
Dx,g cm-3	1.759	1.788
Z	8	8
Mu (mm-1)	2.352	2.353
F000	1912.0	1976.0
F000'	1910.78	
h,k,lmax	42,22,13	41,22,13
Nref	6463	6440
Tmin,Tmax	0.631,0.889	0.648,0.768
Tmin'	0.618	

Correction method= # Reported T Limits: Tmin=0.648 Tmax=0.768  
AbsCorr = GAUSSIAN

Data completeness= 0.996                      Theta(max)= 32.053

R(reflections)= 0.0393( 4949)              wR2(reflections)= 0.1104( 6440)

S = 1.030                                      Npar= 235

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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 B**

PLAT043_ALERT_1_B	Calculated and Reported Mol. Weight Differ by ..	8.06	Check
PLAT213_ALERT_2_B	Atom C018 has ADP max/min Ratio .....	4.2	prolat
PLAT220_ALERT_2_B	Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range	6.4	Ratio
PLAT234_ALERT_4_B	Large Hirshfeld Difference C018 -- C026 ..	0.27	Ang.
PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?) .....	0014	Check
PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?) .....	0013	Check
PLAT430_ALERT_2_B	Short Inter D...A Contact O003 .. O014 ..	2.74	Ang.
PLAT430_ALERT_2_B	Short Inter D...A Contact O005 .. O013 ..	2.81	Ang.
PLAT430_ALERT_2_B	Short Inter D...A Contact O013 .. O013 ..	2.78	Ang.

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**Alert level C**

CHEMW03\_ALERT\_2\_C The ratio of given/expected molecular weight as calculated from the \_atom\_site\* data lies outside the range 0.99 <> 1.01

From the CIF: \_cell\_formula\_units\_Z 8  
From the CIF: \_chemical\_formula\_weight 499.22  
TEST: Calculate formula weight from \_atom\_site\*

atom	mass	num	sum
C	12.01	15.00	180.16
H	1.01	12.00	12.10
O	16.00	10.00	159.99
La	138.91	1.00	138.91

Calculated formula weight 491.16

PLAT041_ALERT_1_C	Calc. and Reported SumFormula Strings Differ	Please	Check
PLAT068_ALERT_1_C	Reported F000 Differs from Calcd (or Missing)...	Please	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C025	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C024	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C019	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	La01	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C010	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C017	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C015	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C026	Check
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds .....	0.00844	Ang.
PLAT410_ALERT_2_C	Short Intra H...H Contact H02C .. H02E ..	1.91	Ang.
PLAT430_ALERT_2_C	Short Inter D...A Contact O004 .. O014 ..	2.89	Ang.
PLAT430_ALERT_2_C	Short Inter D...A Contact O006 .. O013 ..	2.89	Ang.
PLAT430_ALERT_2_C	Short Inter D...A Contact O008 .. O014 ..	2.87	Ang.

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**Alert level G**

FORMU01\_ALERT\_2\_G There is a discrepancy between the atom counts in the \_chemical\_formula\_sum and the formula from the \_atom\_site\* data.

Atom count from \_chemical\_formula\_sum: C15 H20 La1 O10  
Atom count from the \_atom\_site data: C15 H12 La1 O10

CELLZ01\_ALERT\_1\_G Difference between formula and atom\_site contents detected.  
CELLZ01\_ALERT\_1\_G WARNING: H atoms missing from atom site list. Is this intentional?

From the CIF: \_cell\_formula\_units\_Z 8  
From the CIF: \_chemical\_formula\_sum C15 H20 La O10  
TEST: Compare cell contents of formula and atom\_site data

atom	Z*formula	cif sites	diff
C	120.00	120.00	0.00
H	160.00	96.00	64.00
La	8.00	8.00	0.00
O	80.00	80.00	0.00

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	3	Info
PLAT005_ALERT_5_G	No Embedded Refinement Details found in the CIF	Please	Do !
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	10.76	Why ?

PLAT199_ALERT_1_G	Reported _cell_measurement_temperature	..... (K)	293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature	..... (K)	293	Check
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	La01 -- 0005 ..	6.6	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	La01 -- 0009 ..	5.6	s.u.
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	.....	38	Note
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd)	.	1.28	Ratio

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

7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
24 ALERT type 2 Indicator that the structure model may be wrong or deficient  
1 ALERT type 3 Indicator that the structure quality may be low  
3 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 30/03/2016; check.def file version of 30/03/2016**

