

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

| | | | |
|-----------------|---------------------|--------------------|-------------|
| 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

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 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. |

🟡 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. |

🟠 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 -- | O005 .. | 6.6 | s.u. |
| PLAT232_ALERT_2_G | Hirshfeld Test Diff (M-X) La01 -- | O009 .. | 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 |

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

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 30/03/2016; check.def file version of 30/03/2016

