

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Lanthr

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: Lanthr

Bond precision: C-C = 0.0179 Å Wavelength=0.71073

Cell: a=5.0015(6) b=16.944(2) c=11.5374(15)
 alpha=90 beta=92.433(10) gamma=90
Temperature: 293 K

| | Calculated | Reported |
|----------------|-------------|------------|
| Volume | 976.9(2) | 976.9(2) |
| Space group | P 21 | P 21 |
| Hall group | P 2yb | P 2yb |
| Moiety formula | C28 H16 N2 | C28 H16 N2 |
| Sum formula | C28 H16 N2 | C28 H16 N2 |
| Mr | 380.43 | 380.43 |
| Dx,g cm-3 | 1.293 | 1.293 |
| Z | 2 | 2 |
| Mu (mm-1) | 0.076 | 0.076 |
| F000 | 396.0 | 396.0 |
| F000' | 396.14 | |
| h,k,lmax | 6,23,15 | 6,23,15 |
| Nref | 5328[2748] | 5272 |
| Tmin,Tmax | 0.988,0.991 | |
| Tmin' | 0.983 | |

Correction method= Not given

Data completeness= 1.92/0.99 Theta(max)= 29.301

R(reflections)= 0.0799(1378) wR2(reflections)= 0.2388(5272)

S = 0.805 Npar= 271

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 A

| | | |
|-------------------|--|------------|
| PLAT026_ALERT_3_A | Ratio Observed / Unique Reflections (too) Low .. | 26% Check |
| PLAT213_ALERT_2_A | Atom C15 has ADP max/min Ratio | 8.6 oblate |

Alert level B

| | | |
|-------------------|---|--------------|
| PLAT111_ALERT_2_B | ADDSYM Detects New (Pseudo) Centre of Symmetry . | 100 %Fit |
| PLAT112_ALERT_2_B | ADDSYM Detects New (Pseudo) Symm. Elem n | 100 %Fit |
| PLAT113_ALERT_2_B | ADDSYM Suggests Possible Pseudo/New Space Group | P21/n Check |
| PLAT241_ALERT_2_B | High 'MainMol' Ueq as Compared to Neighbors of | C20 Check |
| PLAT340_ALERT_3_B | Low Bond Precision on C-C Bonds | 0.01787 Ang. |
| PLAT930_ALERT_2_B | Check Twin Law (0 0 1) [0 0 1] Estimated BASF | 0.22 |

Alert level C

| | | |
|-------------------|---|--------------|
| RINTA01_ALERT_3_C | The value of Rint is greater than 0.12 | |
| | Rint given 0.157 | |
| STRVA01_ALERT_2_C | Chirality of atom sites is inverted? | |
| | From the CIF: _refine_ls_abs_structure_Flack 6.200 | |
| | From the CIF: _refine_ls_abs_structure_Flack_su 1.000 | |
| PLAT020_ALERT_3_C | The Value of Rint is Greater Than 0.12 | 0.157 Report |
| PLAT213_ALERT_2_C | Atom C19 has ADP max/min Ratio | 3.4 prolat |
| PLAT213_ALERT_2_C | Atom C20 has ADP max/min Ratio | 3.7 prolat |
| PLAT220_ALERT_2_C | Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range | 3.6 Ratio |
| PLAT230_ALERT_2_C | Hirshfeld Test Diff for N1 --C20 . | 7.0 s.u. |
| PLAT230_ALERT_2_C | Hirshfeld Test Diff for C12 --C13 . | 5.1 s.u. |
| PLAT230_ALERT_2_C | Hirshfeld Test Diff for C19 --C20 . | 6.5 s.u. |
| PLAT230_ALERT_2_C | Hirshfeld Test Diff for C26 --C27 . | 6.0 s.u. |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference N1 --C21 | 0.18 Ang. |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference N2 --C27 | 0.19 Ang. |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference N2 --C28 | 0.23 Ang. |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference C1 --C15 | 0.17 Ang. |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference C3 --C4 | 0.21 Ang. |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference C4 --C5 | 0.17 Ang. |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference C5 --C6 | 0.21 Ang. |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference C15 --C16 | 0.16 Ang. |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference C18 --C19 | 0.22 Ang. |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference C22 --C23 | 0.21 Ang. |
| PLAT241_ALERT_2_C | High 'MainMol' Ueq as Compared to Neighbors of | N2 Check |
| PLAT241_ALERT_2_C | High 'MainMol' Ueq as Compared to Neighbors of | C4 Check |
| PLAT241_ALERT_2_C | High 'MainMol' Ueq as Compared to Neighbors of | C6 Check |
| PLAT241_ALERT_2_C | High 'MainMol' Ueq as Compared to Neighbors of | C12 Check |
| PLAT241_ALERT_2_C | High 'MainMol' Ueq as Compared to Neighbors of | C18 Check |
| PLAT241_ALERT_2_C | High 'MainMol' Ueq as Compared to Neighbors of | C26 Check |
| PLAT242_ALERT_2_C | Low 'MainMol' Ueq as Compared to Neighbors of | C13 Check |
| PLAT242_ALERT_2_C | Low 'MainMol' Ueq as Compared to Neighbors of | C17 Check |
| PLAT242_ALERT_2_C | Low 'MainMol' Ueq as Compared to Neighbors of | C19 Check |
| PLAT242_ALERT_2_C | Low 'MainMol' Ueq as Compared to Neighbors of | C27 Check |
| PLAT242_ALERT_2_C | Low 'MainMol' Ueq as Compared to Neighbors of | C28 Check |
| PLAT372_ALERT_2_C | Short C(sp)-C(sp) Bond C15 - C16 . | 1.13 Ang. |
| PLAT906_ALERT_3_C | Large K Value in the Analysis of Variance | 15.216 Check |
| PLAT906_ALERT_3_C | Large K Value in the Analysis of Variance | 4.700 Check |
| PLAT906_ALERT_3_C | Large K Value in the Analysis of Variance | 2.518 Check |
| PLAT907_ALERT_2_C | Flack x > 0.5, Structure Needs to be Inverted? . | 6.20 Check |

Alert level G

| | | |
|-------------------|--|--------------|
| PLAT032_ALERT_4_G | Std. Uncertainty on Flack Parameter Value High . | 1.000 Report |
| PLAT033_ALERT_4_G | Flack x Value Deviates > 3.0 * sigma from Zero . | 6.200 Note |
| PLAT199_ALERT_1_G | Reported _cell_measurement_temperature | 293 Check |
| PLAT200_ALERT_1_G | Reported _diffrn_ambient_temperature | 293 Check |

| | | | | | |
|-------------------|--|-------|-------|-----------|------------|
| PLAT230_ALERT_2_G | Hirshfeld Test Diff for | C8 | --C22 | . | 8.3 s.u. |
| PLAT333_ALERT_2_G | Large Aver C6-Ring C-C Dist. | C1 | -C14 | | 1.42 Ang. |
| PLAT335_ALERT_2_G | Check Large C6 Ring C-C Range | C2 | -C7 | | 0.20 Ang. |
| PLAT371_ALERT_2_G | Long C(sp2)-C(sp1) Bond | C1 | -C15 | . | 1.46 Ang. |
| PLAT371_ALERT_2_G | Long C(sp2)-C(sp1) Bond | C16 | -C17 | . | 1.48 Ang. |
| PLAT870_ALERT_4_G | ALERTS Related to Twinning Effects Suppressed | .. | | | ! Info |
| PLAT912_ALERT_4_G | Missing # of FCF Reflections Above STh/L= | 0.600 | | | 22 Note |
| PLAT916_ALERT_2_G | Hooft y and Flack x Parameter Values Differ by | . | | | 5.35 Check |
| PLAT931_ALERT_5_G | Found Twin Law (0 0 1) [| |] | Est. BASF | 0.22 Check |

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

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
33 ALERT type 2 Indicator that the structure model may be wrong or deficient
7 ALERT type 3 Indicator that the structure quality may be low
14 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.

PLATON version of 23/04/2018; check.def file version of 23/04/2018

