

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) exp\_458

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: exp\_458

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|                 |                         |                         |              |
|-----------------|-------------------------|-------------------------|--------------|
| Bond precision: | C-C = 0.0142 Å          | Wavelength=1.54184      |              |
| Cell:           | a=17.8192(4)            | b=16.9757(5)            | c=17.5726(4) |
|                 | alpha=90                | beta=90                 | gamma=90     |
| Temperature:    | 100 K                   |                         |              |
|                 | Calculated              | Reported                |              |
| Volume          | 5315.6(2)               | 5315.6(2)               |              |
| Space group     | P n a 21                | P n a 21                |              |
| Hall group      | P 2c -2n                | P 2c -2n                |              |
| Moiety formula  | C24 B F20, C32 H55 Dy P | C32 H55 Dy P, B C24 F20 |              |
| Sum formula     | C56 H55 B Dy F20 P      | C56 H55 B Dy F20 P      |              |
| Mr              | 1312.28                 | 1312.28                 |              |
| Dx,g cm-3       | 1.640                   | 1.640                   |              |
| Z               | 4                       | 4                       |              |
| Mu (mm-1)       | 8.778                   | 8.778                   |              |
| F000            | 2628.0                  | 2628.0                  |              |
| F000'           | 2599.92                 |                         |              |
| h,k,lmax        | 21,20,20                | 21,20,20                |              |
| Nref            | 9482[ 4911]             | 9379                    |              |
| Tmin,Tmax       | 0.520,0.645             | 0.649,1.000             |              |
| Tmin'           | 0.472                   |                         |              |

Correction method= # Reported T Limits: Tmin=0.649 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 1.91/0.99      Theta(max)= 67.070

R(reflections)= 0.0562( 8005)      wR2(reflections)= 0.1561( 9379)

S = 1.033      Npar= 781

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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.



### Alert level C

|                   |  |         |        |
|-------------------|--|---------|--------|
| PLAT090_ALERT_3_C | Poor Data / Parameter Ratio (Zmax > 18) .....  | 6.27    | Note   |
| PLAT241_ALERT_2_C | High 'MainMol' Ueq as Compared to Neighbors of | C7      | Check  |
| 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 | C13     | Check  |
| PLAT241_ALERT_2_C | High 'MainMol' Ueq as Compared to Neighbors of | C14     | Check  |
| PLAT241_ALERT_2_C | High 'MainMol' Ueq as Compared to Neighbors of | C16     | Check  |
| PLAT241_ALERT_2_C | High 'MainMol' Ueq as Compared to Neighbors of | C17     | Check  |
| PLAT241_ALERT_2_C | High 'MainMol' Ueq as Compared to Neighbors of | C19     | Check  |
| PLAT241_ALERT_2_C | High 'MainMol' Ueq as Compared to Neighbors of | C20     | Check  |
| PLAT334_ALERT_2_C | Small Aver. Benzene C-C Dist C33 -C38          | 1.37    | Ang.   |
| PLAT342_ALERT_3_C | Low Bond Precision on C-C Bonds .....          | 0.01425 | Ang.   |
| PLAT911_ALERT_3_C | Missing FCF Refl Between Thmin & STh/L= 0.597  | 16      | Report |



### Alert level G

|                   |  |        |        |
|-------------------|--|--------|--------|
| PLAT002_ALERT_2_G | Number of Distance or Angle Restraints on AtSite | 21     | 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  |
| PLAT172_ALERT_4_G | The CIF-Embedded .res File Contains DFIX Records | 8      | Report |
| PLAT177_ALERT_4_G | The CIF-Embedded .res File Contains DELU Records | 1      | Report |
| PLAT186_ALERT_4_G | The CIF-Embedded .res File Contains ISOR Records | 3      | Report |
| PLAT232_ALERT_2_G | Hirshfeld Test Diff (M-X) Dyl --P1               | 6.3    | s.u.   |
| PLAT302_ALERT_4_G | Anion/Solvent/Minor-Residue Disorder (Resd 2 )   | 18%    | Note   |
| PLAT328_ALERT_4_G | Possible Missing H on sp3? Phosphorus .....      | P1     | Check  |
| PLAT367_ALERT_2_G | Long? C(sp?)-C(sp?) Bond C21 - C25               | 1.50   | Ang.   |
| PLAT367_ALERT_2_G | Long? C(sp?)-C(sp?) Bond C23 - C29               | 1.52   | Ang.   |
| PLAT367_ALERT_2_G | Long? C(sp?)-C(sp?) Bond C24 - C31               | 1.53   | Ang.   |
| PLAT412_ALERT_2_G | Short Intra XH3 .. XHn H25B ..H20A               | 2.13   | Ang.   |
|                   | x,y,z =  | 1_555  | Check  |
| PLAT434_ALERT_2_G | Short Inter HL..HL Contact F4 ..F9               | 2.66   | Ang.   |
|                   | 1-x,1-y,-1/2+z =                                 | 2_664  | Check  |
| PLAT434_ALERT_2_G | Short Inter HL..HL Contact F13 ..F17             | 2.76   | Ang.   |
|                   | 1/2-x,-1/2+y,1/2+z =                             | 4_545  | Check  |
| PLAT720_ALERT_4_G | Number of Unusual/Non-Standard Labels .....      | 12     | Note   |
| PLAT860_ALERT_3_G | Number of Least-Squares Restraints .....         | 42     | Note   |
| PLAT909_ALERT_3_G | Percentage of I>2sig(I) Data at Theta(Max) Still | 54%    | Note   |
| PLAT933_ALERT_2_G | Number of OMIT Records in Embedded .res File ... | 2      | Note   |
| PLAT978_ALERT_2_G | Number C-C Bonds with Positive Residual Density. | 0      | Info   |

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain  
0 **ALERT level B** = A potentially serious problem, consider carefully  
12 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
20 **ALERT level G** = General information/check it is not something unexpected
- 1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
20 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  
6 ALERT type 4 Improvement, methodology, query or suggestion  
0 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.

