# checkCIF/PLATON report

**No syntax errors found.** **CIF dictionary** **Interpreting this report**

# Datablock: char083

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**Bond precision: C-C = 0.0221 A Wavelength=0.71073**

**Cell: a=15.147(3) b=11.447(2) c=18.383(4)**
**alpha=90 beta=90.05(5) gamma=90**

| | Calculated | Reported |
|---|---|---|
| Volume | 3187.4(11) | 3187.4(11) |
| Space group | P 21/c | P2(1)/c |
| Hall group | -P 2ybc | ? |
| Moiety formula | C27 H53 B Co P S3 | ? |
| Sum formula | C27 H53 B Co P S3 | C27 H53 B Co P S3 |
| Mr | 574.61 | 574.58 |
| Dx,g cm-3 | 1.197 | 1.197 |
| Z | 4 | 4 |
| Mu (mm-1) | 0.799 | 0.799 |
| F000 | 1240.0 | 1240.0 |
| F000' | 1243.53 | |
| h,k,lmax | 15,12,19 | 15,12,19 |
| Nref | 3886 | 3849 |
| Tmin,Tmax | 0.852,0.866 | 0.857,0.869 |
| Tmin' | 0.852 | |

**Correction method= AbsCorr=MULTI-SCAN**

**Data completeness= Ratio = 0.990 Theta(max)= 21.990**

**R(reflections)= 0.0851( 3143) wR2(reflections)= 0.2206( 3849)**

**S = 1.012 Npar= 287**

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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 A**

THETM01_ALERT_3_A The value of sine(theta_max)/wavelength is less than 0.550
Calculated sin(theta_max)/wavelength = 0.5268
PLAT027_ALERT_3_A _diffrn_reflns_theta_full (too) Low ..... 21.99 Deg.
PLAT213_ALERT_2_A Atom C2 has ADP max/min Ratio ..... 6.20 prola
PLAT213_ALERT_2_A Atom C3 has ADP max/min Ratio ..... 14.80 prola
PLAT213_ALERT_2_A Atom C19 has ADP max/min Ratio ..... 5.40 prola
PLAT213_ALERT_2_A Atom C23 has ADP max/min Ratio ..... 7.90 prola

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PLAT213_ALERT_2_A Atom C25     has ADP max/min Ratio .............       8.10 prola
PLAT220_ALERT_2_A Large Non-Solvent    C     Ueq(max)/Ueq(min) ...       5.20 Ratio
PLAT222_ALERT_3_A Large Non-Solvent    H     Ueq(max)/Ueq(min) ...       5.51 Ratio
PLAT242_ALERT_2_A Check Low       Ueq as Compared to Neighbors for        C22
PLAT360_ALERT_2_A Short  C(sp3)-C(sp3) Bond  C22    -   C23    ...       1.09 Ang.
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## Alert level B

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PLAT213_ALERT_2_B Atom C5      has ADP max/min Ratio .............       5.00 prola
PLAT213_ALERT_2_B Atom C6      has ADP max/min Ratio .............       4.20 prola
PLAT213_ALERT_2_B Atom C22     has ADP max/min Ratio .............       4.20 prola
PLAT242_ALERT_2_B Check Low       Ueq as Compared to Neighbors for        C18
PLAT341_ALERT_3_B Low Bond Precision on C-C Bonds (x 1000) Ang ...         22
PLAT413_ALERT_2_B Short Inter XH3 .. XHn     H3A    ..  H19A    ..       2.06 Ang.
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## Alert level C

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PLAT213_ALERT_2_C Atom S3      has ADP max/min Ratio .............       3.20 prola
PLAT213_ALERT_2_C Atom C1      has ADP max/min Ratio .............       3.90 prola
PLAT213_ALERT_2_C Atom C4      has ADP max/min Ratio .............       3.70 prola
PLAT213_ALERT_2_C Atom C7      has ADP max/min Ratio .............       3.10 prola
PLAT213_ALERT_2_C Atom C18     has ADP max/min Ratio .............       3.30 prola
PLAT213_ALERT_2_C Atom C21     has ADP max/min Ratio .............       3.60 prola
PLAT213_ALERT_2_C Atom C24     has ADP max/min Ratio .............       4.00 prola
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for         C2
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for        C17
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for          P
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....       3.12
PLAT320_ALERT_2_C Check Hybridisation of  C22    in Main Residue .          ?
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## Alert level G

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PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints .......        283
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  11 ALERT level A = In general: serious problem
   6 ALERT level B = Potentially serious problem
  12 ALERT level C = Check and explain
   1 ALERT level G = General alerts; check

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  25 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
   0 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
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**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*, 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 27/11/2007; check.def file version of 27/11/2007**

## Datablock char083 - ellipsoid plot