

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 3-Pr

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: 3-Pr

Bond precision: C-C = 0.0104 Å

Wavelength=1.54184

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Cell:      a=11.4811(3)
           alpha=85.159(3)
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b=13.1643 (5) c=20.9850 (7)
beta=75.596 (2) gamma=68.108 (3)

Temperature: 120 K

| | Calculated |
|------------------------|------------------|
| Volume | 2850.34 (17) |
| Space group | P -1 |
| Hall group | -P 1 |
| Moiety formula | C56 H89 O4 P4 Pr |
| Sum formula | C56 H89 O4 P4 Pr |
| Mr | 1091.07 |
| Dx, g cm ⁻³ | 1.271 |
| Z | 2 |
| Mu (mm ⁻¹) | 7.931 |
| F000 | 1152.0 |
| F000' | 1152.09 |
| h, k, lmax | 14, 16, 26 |
| Nref | 12518 |
| Tmin, Tmax | 0.423, 0.471 |
| Tmin' | 0.191 |

```
Reported
2850.34 (17)
P -1
-P 1
C56 H89 O4 P4 Pr
C56 H89 O4 P4 Pr
1091.06
1.271
2
7.931
1152.0

14,16,26
12203
0.402,1.000
```

Correction method= # Reported T Limits: Tmin=0.402 Tmax=1.000
AbsCorr = MULTI-SCAN

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Data completeness= 0.975
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$$\text{Theta (max)} = 80.559$$

R(reflections)= 0.0740(10480)

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wR2 (reflections)=  
0.1880 ( 12203)
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$$S = 1.073$$

Npar= 911

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

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 0.75Ang From Pr1 3.86 eA-3

Author Response: This could not be modelled as any chemically sensible species and it is due to the proximity of a strong absorber (Pr).

Alert level B

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 0.80Ang From Pr1 2.76 eA-3

Author Response: This could not be modelled as any chemically sensible species and it is due to the proximity of a strong absorber (Pr).

PLAT973_ALERT_2_B Check Calcd Positive Resid. Density on Pr1 1.98 eA-3

Author Response: This could not be modelled as any chemically sensible species and it is due to the proximity of a strong absorber (Pr).

Alert level C

PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density 2.05 Report
PLAT213_ALERT_2_C Atom C10A has ADP max/min Ratio 3.1 oblate
PLAT213_ALERT_2_C Atom C13A has ADP max/min Ratio 3.8 oblate
PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 4.0 Ratio
PLAT220_ALERT_2_C NonSolvent Resd 1 O Ueq(max)/Ueq(min) Range 3.2 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 4.3 Ratio
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of 03 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C31 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C34 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C29 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C30 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C33 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C35 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C39 Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds 0.01037 Ang.
PLAT601_ALERT_2_C Unit Cell Contains Solvent Accessible VOIDS of . 31 Ang**3
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 2.541 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 22 Report
1 0 0, -12 1 0, 1 1 0, -11 3 0, 11 -3 1, -1 -1 1,
12 -1 1, -6 1 1, 1 2 1, -11 3 1, 11 -3 2, 12 -1 2,
0 0 2, -11 3 2, 11 -4 3, 11 -3 3, 11 -4 4, 12 -2 4,
11 -4 5, 12 -2 5, 3 2 5, 6 10 15,
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.10Ang From Pr1 -2.04 eA-3

● **Alert level G**

| | | | |
|-------------------|--|---------|-------------|
| PLAT002_ALERT_2_G | Number of Distance or Angle Restraints on AtSite | 65 | Note |
| PLAT003_ALERT_2_G | Number of Uiso or U(i,j) Restrained non-H Atoms | 64 | Report |
| PLAT007_ALERT_5_G | Number of Unrefined Donor-H Atoms | 2 | Report |
| | H1 H4A | | |
| PLAT083_ALERT_2_G | SHELXL Second Parameter in WGHT Unusually Large | 7.53 | Why ? |
| PLAT175_ALERT_4_G | The CIF-Embedded .res File Contains SAME Records | 3 | Report |
| PLAT176_ALERT_4_G | The CIF-Embedded .res File Contains SADI Records | 1 | Report |
| PLAT178_ALERT_4_G | The CIF-Embedded .res File Contains SIMU Records | 1 | Report |
| PLAT188_ALERT_3_G | A Non-default SIMU Restraint Value has been used | 0.0100 | Report |
| PLAT232_ALERT_2_G | Hirshfeld Test Diff (M-X) Pr1 --O4 . | 5.7 | s.u. |
| PLAT232_ALERT_2_G | Hirshfeld Test Diff (M-X) Pr1 --O4A . | 6.6 | s.u. |
| PLAT301_ALERT_3_G | Main Residue Disorder(Resd 1) | 49% | Note |
| PLAT412_ALERT_2_G | Short Intra XH3 .. XHn H24B ..H50A . | 2.10 | Ang. |
| | | x,y,z = | 1_555 Check |
| PLAT720_ALERT_4_G | Number of Unusual/Non-Standard Labels | 7 | Note |
| | H4AA H8AA H8AB H8AC H9AA H9AB H9AC | | |
| PLAT802_ALERT_4_G | CIF Input Record(s) with more than 80 Characters | 2 | Info |
| PLAT811_ALERT_5_G | No ADDSYM Analysis: Too Many Excluded Atoms | ! | Info |
| PLAT860_ALERT_3_G | Number of Least-Squares Restraints | 1183 | Note |
| PLAT912_ALERT_4_G | Missing # of FCF Reflections Above STh/L= 0.600 | 293 | Note |
| PLAT933_ALERT_2_G | Number of HKL-OMIT Records in Embedded .res File | 6 | Note |
| | -1 -1 1, 0 0 2, 1 0 0, 1 1 0, 1 2 1, 3 2 5, | | |
| PLAT969_ALERT_5_G | The 'Henn et al.' R-Factor-gap value | 3.081 | Note |
| | Predicted wR2: Based on SigI**2 6.10 or SHELX Weight 17.52 | | |
| PLAT978_ALERT_2_G | Number C-C Bonds with Positive Residual Density. | 0 | Info |

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- 1 **ALERT level A** = Most likely a serious problem - resolve or explain
2 **ALERT level B** = A potentially serious problem, consider carefully
19 **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

- 0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
26 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
6 ALERT type 4 Improvement, methodology, query or suggestion
3 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.

