

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) vv3pr

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: vv3pr

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Bond precision:    C-C = 0.0040 Å                      Wavelength=0.71073

Cell:                      a=11.533(2)              b=27.173(5)              c=6.0720(12)  
                                alpha=90              beta=118.04(3)              gamma=90

Temperature:              100 K

	Calculated	Reported
Volume	1679.5(7)	1679.5(7)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	C15 H13 O11 Pr	C15 H13 O11 Pr
Sum formula	C15 H13 O11 Pr	C15 H13 O11 Pr
Mr	510.16	510.16
Dx, g cm <sup>-3</sup>	2.018	2.018
Z	4	4
Mu (mm <sup>-1</sup> )	2.962	2.962
F000	1000.0	1000.0
F000'	999.71	
h, k, lmax	13, 32, 7	13, 32, 6
Nref	1499	1449
Tmin, Tmax	0.808, 0.942	
Tmin'	0.744	

Correction method= Not given

Data completeness= 0.967                      Theta(max)= 25.024

R(reflections)= 0.0179( 1438)

wR2(reflections)=  
0.0468( 1449)

S = 1.097

Npar= 143

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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 C

PLAT029_ALERT_3_C	_diffn_measured_fraction_theta_full value Low	0.966	Why?
PLAT057_ALERT_3_C	Correction for Absorption Required RT(exp) ...	1.17	Do !
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.595	32	Report
PLAT976_ALERT_2_C	Check Calcd Resid. Dens. 1.07Ang From O4	-0.44	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H4A	-0.32	eA-3

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### Alert level G

ABSMU01_ALERT_1_G	Calculation of _exptl_absorpt_correction_mu not performed for this radiation type.		
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	4	Report
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	2	Info
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms .....	2	Report
PLAT128_ALERT_4_G	Alternate Setting for Input Space Group C2/c	I2/a	Note
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	1	Report
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Pr1 --O4	5.8	s.u.
PLAT300_ALERT_4_G	Atom Site Occupancy of O6 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C8 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C9 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C10 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H8 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H9 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H10 Constrained at	0.5	Check
PLAT301_ALERT_3_G	Main Residue Disorder .....(Resd 1 )	14%	Note
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O3	106.4	Degree
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O6	107.1	Degree
PLAT767_ALERT_4_G	INS Embedded LIST 6 Instruction Should be LIST 4		Please Check
PLAT789_ALERT_4_G	Atoms with Negative _atom_site_disorder_group #	7	Check
PLAT794_ALERT_5_G	Tentative Bond Valency for Pr1 (III)	3.36	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....	18	Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary		Please Do !
PLAT909_ALERT_3_G	Percentage of I>2sig(I) Data at Theta(Max) Still	98%	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	4	Info

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- 0 **ALERT level A** = Most likely a serious problem - resolve or explain  
0 **ALERT level B** = A potentially serious problem, consider carefully  
5 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
24 **ALERT level G** = General information/check it is not something unexpected
- 2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
7 ALERT type 2 Indicator that the structure model may be wrong or deficient  
6 ALERT type 3 Indicator that the structure quality may be low  
11 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.

