

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) prterpytry1

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: prterpytry1

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Bond precision:      C-C = 0.0051 Å

Wavelength=0.71073

Cell:                      a=11.1709(3)                      b=16.0121(4)                      c=16.2966(4)  
                              alpha=106.743(1)                      beta=94.995(1)                      gamma=95.845(1)  
Temperature:              300 K

	Calculated	Reported
Volume	2756.07(12)	2756.07(12)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C30 H22 N8 O6 Pr, C15 H11 N7 O12 Pr, 2(C2 H3 N)	C30 H22 N8 O6 Pr, C15 H11 N7 O12 Pr, 2(C2 H3 N)
Sum formula	C49 H39 N17 O18 Pr2	C49 H39 N17 O18 Pr2
Mr	1435.79	1435.79
Dx, g cm <sup>-3</sup>	1.730	1.730
Z	2	2
Mu (mm <sup>-1</sup> )	1.836	1.836
F000	1428.0	2592.0
F000'	1427.73	
h,k,lmax	16,23,23	16,23,23
Nref	17607	16986
Tmin,Tmax	0.583,0.748	0.607,0.746
Tmin'	0.572	

Correction method= # Reported T Limits: Tmin=0.607 Tmax=0.746  
AbsCorr = MULTI-SCAN

Data completeness= 0.965

Theta(max)= 31.030

R(reflections)= 0.0373( 13026)

wR2(reflections)=  
0.0828( 16986)

S = 1.014

Npar= 893

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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 B

PLAT242\_ALERT\_2\_B Low 'MainMol' Ueq as Compared to Neighbors of N15 Check  
PLAT913\_ALERT\_3\_B Missing # of Very Strong Reflections in FCF .... 205 Note

1	0	0,	5	0	0,	-4	1	0,	1	1	0,	4	1	0,	5	2	0,
-2	3	0,	-1	3	0,	0	4	0,	1	4	0,	-6	5	0,	-3	5	0,
0	5	0,	2	5	0,	-2	6	0,	-1	7	0,	0	7	0,	1	8	0,
-1	-8	1,	2	-8	1,	-2	-7	1,	3	-7	1,	-1	-6	1,	0	-6	1,

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### Alert level C

PLAT068\_ALERT\_1\_C Reported F000 Differs from Calcd (or Missing)... Please Check  
PLAT220\_ALERT\_2\_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.1 Ratio  
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 O14 Check  
PLAT241\_ALERT\_2\_C High 'MainMol' Ueq as Compared to Neighbors of O16 Check  
PLAT242\_ALERT\_2\_C Low 'MainMol' Ueq as Compared to Neighbors of Pr2 Check  
PLAT242\_ALERT\_2\_C Low 'MainMol' Ueq as Compared to Neighbors of N12 Check  
PLAT244\_ALERT\_4\_C Low 'Solvent' Ueq as Compared to Neighbors of C46 Check  
PLAT244\_ALERT\_4\_C Low 'Solvent' Ueq as Compared to Neighbors of C48 Check  
PLAT245\_ALERT\_2\_C U(iso) H14 Smaller than U(eq) C14 by 0.011 Ang\*\*2  
PLAT245\_ALERT\_2\_C U(iso) H34 Smaller than U(eq) C34 by 0.019 Ang\*\*2  
PLAT260\_ALERT\_2\_C Large Average Ueq of Residue Including N17 0.112 Check  
PLAT410\_ALERT\_2\_C Short Intra H...H Contact H4 ..H7 . 1.99 Ang.

x,y,z = 1\_555 Check

PLAT911\_ALERT\_3\_C Missing FCF Refl Between Thmin & STh/L= 0.600 486 Report

3	0	0,	5	0	0,	-6	1	0,	-4	1	0,	-2	1	0,	1	1	0,
2	1	0,	4	1	0,	-2	2	0,	1	2	0,	3	2	0,	5	2	0,
-6	3	0,	-4	3	0,	-2	3	0,	-1	3	0,	0	3	0,	4	3	0,
7	3	0,	-5	4	0,	-3	4	0,	0	4	0,	1	4	0,	3	4	0,
-6	5	0,	-3	5	0,	0	5	0,	2	5	0,	-2	6	0,	3	6	0,
-1	7	0,	0	7	0,	2	7	0,	-4	8	0,	1	8	0,	2	8	0,
-1	-8	1,	2	-8	1,	-4	-7	1,	-2	-7	1,	0	-7	1,	3	-7	1,
4	-7	1,	-3	-6	1,	-1	-6	1,	0	-6	1,	4	-6	1,	-4	-5	1,
-2	-5	1,	1	-5	1,	4	-5	1,	-6	-4	1,	-5	-4	1,	-3	-4	1,
-1	-4	1,	0	-4	1,	1	-4	1,	2	-4	1,	-4	-3	1,	-1	-3	1,
0	-3	1,	2	-3	1,	4	-3	1,	-5	-2	1,	-4	-2	1,	-3	-2	1,
-2	-2	1,	-1	-2	1,	0	-2	1,	1	-2	1,	5	-2	1,	-6	-1	1,
-4	-1	1,	-3	-1	1,	-2	-1	1,	1	-1	1,	2	-1	1,	3	-1	1,
4	-1	1,	-5	0	1,	-3	0	1,	-2	0	1,	1	0	1,	2	0	1,
3	0	1,	-4	1	1,	-1	1	1,	0	1	1,	1	1	1,	4	1	1,
7	1	1,	-2	2	1,	-1	2	1,	0	2	1,	1	2	1,	3	2	1,

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### Alert level G

PLAT012\_ALERT\_1\_G No \_shelx\_res\_checksum Found in CIF ..... Please Check  
PLAT019\_ALERT\_1\_G \_diffn\_measured\_fraction\_theta\_full/\*\_max < 1.0 0.985 Report  
PLAT154\_ALERT\_1\_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.001 Degree  
PLAT164\_ALERT\_4\_G Nr. of Refined C-H H-Atoms in Heavy-Atom Struct. 29 Note  
PLAT232\_ALERT\_2\_G Hirshfeld Test Diff (M-X) Pr1 --O1 . 8.2 s.u.  
PLAT232\_ALERT\_2\_G Hirshfeld Test Diff (M-X) Pr1 --O2 . 5.5 s.u.

PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Pr1	--O4	.	6.4 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Pr1	--O5	.	6.7 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Pr2	--O10	.	9.4 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Pr2	--O11	.	6.8 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Pr2	--O13	.	8.1 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Pr2	--O14	.	11.3 s.u.
PLAT794_ALERT_5_G	Tentative Bond Valency for Pr1	(III)	.	3.96	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Pr2	(III)	.	3.97	Info
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).				4 Note
	1 0 0, 0 1 0, 0 -1 1, 0 0 1,				
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600				130 Note
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value .....				1.396 Note
	Predicted wR2: Based on SigI**2 5.93 or SHELX Weight 8.17				
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.				2 Info

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

4 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  
 3 ALERT type 3 Indicator that the structure quality may be low  
 4 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.

