

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) rf1933

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: rf1933

Bond precision:	C-C = 0.0023 A	Wavelength=0.71073
Cell:	a=13.2021(5)	b=14.6509(6) c=24.8108(10)
	alpha=90	beta=98.938(2) gamma=90
Temperature:	100 K	
	Calculated	Reported
Volume	4740.7(3)	4740.7(3)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C54 H36 F9 N2 O8 Pr	C54 H36 F9 N2 O8 Pr
Sum formula	C54 H36 F9 N2 O8 Pr	C54 H36 F9 N2 O8 Pr
Mr	1152.76	1152.76
Dx,g cm-3	1.615	1.615
Z	4	4
Mu (mm-1)	1.123	1.123
F000	2312.0	2312.0
F000'	2312.54	
h,k,lmax	18,21,35	18,20,35
Nref	14638	14586
Tmin,Tmax	0.785,0.884	0.754,0.910
Tmin'	0.781	
Correction method= # Reported T Limits: Tmin=0.754 Tmax=0.910		
AbsCorr = MULTI-SCAN		
Data completeness=	0.996	Theta(max)= 30.641
R(reflections)=	0.0260(13656)	wR2(reflections)= 0.0622(14586)
S =	1.146	Npar= 669

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

PLAT213_ALERT_2_C	Atom F4	has ADP max/min Ratio	3.4	prolat
PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of	C15	Check
PLAT601_ALERT_2_C	Unit Cell Contains Solvent Accessible VOIDS of	.	45	Ang**3



Alert level G

PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT	Unusually Large	6.41	Why ?
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Pr1	--O3 .	5.4	s.u.
PLAT794_ALERT_5_G	Tentative Bond Valency for Pr1	(III) .	3.57	Info
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary	.		Please Do !
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600	51	Note
PLAT965_ALERT_2_G	The SHELXL WEIGHT Optimisation has not Converged			Please Check
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		16	Info

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

1 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
 0 ALERT type 3 Indicator that the structure quality may be low
 1 ALERT type 4 Improvement, methodology, query or suggestion
 1 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.

Datablock rf1933 - ellipsoid plot

