

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) b-2-41

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: b-2-41

Bond precision:	C-C = 0.0048 A	Wavelength=1.54184
Cell:	a=10.3471(8) b=19.4565(10) c=14.7658(9)	
	alpha=90 beta=107.958(7) gamma=90	
Temperature:	293 K	
	Calculated	Reported
Volume	2827.8(3)	2827.8(3)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C31 H22 N3 O4 P [+ solvent]	C31 H22 N3 O4 P
Sum formula	C31 H22 N3 O4 P [+ solvent]	C31 H22 N3 O4 P
Mr	531.49	531.48
Dx, g cm ⁻³	1.248	1.248
Z	4	4
Mu (mm ⁻¹)	1.191	1.191
F000	1104.0	1104.0
F000'	1108.41	
h,k,lmax	12,23,17	12,23,17
Nref	5154	5006
Tmin,Tmax	0.752,0.797	0.578,1.000
Tmin'	0.682	

Correction method= # Reported T Limits: Tmin=0.578 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.971 Theta(max)= 67.938

R(reflections)= 0.0528(3517) wR2(reflections)= 0.1591(5006)

S = 1.035 Npar= 352

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**

PLAT029_ALERT_3_C	_diffrn_measured_fraction_theta_full	value Low	.	0.976	Why?
PLAT241_ALERT_2_C	High	MainMol Ueq as Compared to Neighbors of		C14	Check
PLAT241_ALERT_2_C	High	MainMol Ueq as Compared to Neighbors of		C18	Check
PLAT241_ALERT_2_C	High	MainMol Ueq as Compared to Neighbors of		C19	Check
PLAT241_ALERT_2_C	High	MainMol Ueq as Compared to Neighbors of		C27	Check
PLAT241_ALERT_2_C	High	MainMol Ueq as Compared to Neighbors of		C28	Check
PLAT242_ALERT_2_C	Low	MainMol Ueq as Compared to Neighbors of		N2	Check
PLAT242_ALERT_2_C	Low	MainMol Ueq as Compared to Neighbors of		C26	Check
PLAT242_ALERT_2_C	Low	MainMol Ueq as Compared to Neighbors of		C29	Check
PLAT331_ALERT_2_C	Small Aver	Phenyl C-C Dist C26 --C31	.	1.37	Ang.
PLAT340_ALERT_3_C	Low Bond Precision on	C-C Bonds	0.00481	Ang.
PLAT911_ALERT_3_C	Missing FCF Refl Between	Thmin & STh/L=	0.600	122	Report

● **Alert level G**

PLAT199_ALERT_1_G	Reported	_cell_measurement_temperature (K)	293	Check
PLAT200_ALERT_1_G	Reported	_diffrn_ambient_temperature (K)	293	Check
PLAT605_ALERT_4_G	Largest Solvent Accessible VOID in the Structure			162	A**3
PLAT868_ALERT_4_G	ALERTS Due to the Use of	_smtbx_masks Suppressed		!	Info
PLAT909_ALERT_3_G	Percentage of I>2sig(I) Data at Theta(Max) Still			41%	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above	STh/L=	0.600	27	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.			1	Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain

0 **ALERT level B** = A potentially serious problem, consider carefully

12 **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

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

10 ALERT type 2 Indicator that the structure model may be wrong or deficient

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

3 ALERT type 4 Improvement, methodology, query or suggestion

0 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.

PLATON version of 22/12/2019; check.def file version of 13/12/2019

