

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: s2601lm_sq

Bond precision:	C-C = 0.0146 A	Wavelength=0.71073
Cell:	a=12.1254(10)	b=13.9304(12) c=40.007(3)
	alpha=90	beta=93.564(4) gamma=90
Temperature:	130 K	
	Calculated	Reported
Volume	6744.6(10)	6744.6(10)
Space group	P 21/n	P 21/n
Hall group	: -P 2yn	-P 2yn
Moiety formula	C64 H48 Cu N4 O P2, F6 P, C H2 Cl2 [+ solvent]	C64 H48 Cu N4 O P2, F6 P, C H2 Cl2
Sum formula	C65 H50 Cl2 Cu F6 N4 O P3 [+ solvent]	C65 H50 Cl2 Cu F6 N4 O P3
Mr	1244.45	1244.44
Dx, g cm-3	1.226	1.226
Z	4	4
Mu (mm-1)	0.532	0.532
F000	2552.0	2552.0
F000'	2556.73	
h,k,lmax	14,16,48	14,16,48
Nref	12525	12284
Tmin,Tmax	0.873,0.905	0.480,0.728
Tmin'	0.850	

Correction method= # Reported T Limits: Tmin=0.480 Tmax=0.728
AbsCorr = NUMERICAL

Data completeness= 0.981 Theta(max)= 25.473

R(reflections)= 0.1232(6409) wR2(reflections)= 0.2824(12284)

S = 1.047 Npar= 741

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 B

PLAT260_ALERT_2_B Large Average Ueq of Residue Including P3 0.167 Check

● Alert level C

PLAT082_ALERT_2_C	High R1 Value	0.12	Report
PLAT084_ALERT_3_C	High wR2 Value (i.e. > 0.25)	0.28	Report
PLAT220_ALERT_2_C	Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range	3.1	Ratio
PLAT230_ALERT_2_C	Hirshfeld Test Diff for C61 --C62 .	5.1	s.u.
PLAT234_ALERT_4_C	Large Hirshfeld Difference P2 --C53 .	0.16	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference N3 --C13 .	0.18	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C7 --C8 .	0.17	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C9 --C10 .	0.16	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C15 --C16 .	0.17	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C18 --C19 .	0.20	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C23 --C24 .	0.19	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C32 --C33 .	0.19	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C32 --C34 .	0.18	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C49 --C50 .	0.16	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C53 --C58 .	0.22	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C54 --C55 .	0.17	Ang.
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of C8		Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of C51		Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of C58		Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of C61		Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of C47		Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of C53		Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of C1X		Check
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor ...	2.3	Note
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including C11X	0.138	Check
PLAT341_ALERT_3_C	Low Bond Precision on C-C Bonds	0.01462	Ang.

● Alert level G

PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	9	Report
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	58.00	Why ?
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records	2	Report
PLAT244_ALERT_4_G	Low 'Solvent' Ueq as Compared to Neighbors of	P3	Check
PLAT606_ALERT_4_G	VERY LARGE Solvent Accessible VOID(S) in Structure	!	Info
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	2	Note
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	54	Note
PLAT869_ALERT_4_G	ALERTS Related to the Use of SQUEEZE Suppressed	!	Info
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	2	Note

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

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

26 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

9 **ALERT level G** = General information/check it is not something unexpected

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

15 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

18 ALERT type 4 Improvement, methodology, query or suggestion

0 ALERT type 5 Informative message, check

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PLAT082_s26011m_sq
;
PROBLEM: High R1 Value ..... 0.12 Report
RESPONSE: ...
;
_vrf_PLAT084_s26011m_sq
;
PROBLEM: High wR2 Value (i.e. > 0.25) ..... 0.28 Report
RESPONSE: ...
;
_vrf_PLAT220_s26011m_sq
;
PROBLEM: Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 3.1 Ratio
RESPONSE: ...
;
_vrf_PLAT230_s26011m_sq
;
PROBLEM: Hirshfeld Test Diff for C61 --C62 . 5.1 s.u.
RESPONSE: ...
;
_vrf_PLAT234_s26011m_sq
;
PROBLEM: Large Hirshfeld Difference P2 --C53 . 0.16 Ang.
RESPONSE: ...
;
_vrf_PLAT241_s26011m_sq
;
PROBLEM: High 'MainMol' Ueq as Compared to Neighbors of C8 Check
RESPONSE: ...
;
_vrf_PLAT242_s26011m_sq
;
PROBLEM: Low 'MainMol' Ueq as Compared to Neighbors of C47 Check
RESPONSE: ...
;
_vrf_PLAT244_s26011m_sq
;
PROBLEM: Low 'Solvent' Ueq as Compared to Neighbors of C1X Check
RESPONSE: ...
;
_vrf_PLAT250_s26011m_sq
;
PROBLEM: Large U3/U1 Ratio for Average U(i,j) Tensor .... 2.3 Note
RESPONSE: ...
;
_vrf_PLAT260_s26011m_sq
;
PROBLEM: Large Average Ueq of Residue Including C11X 0.138 Check
RESPONSE: ...
;
_vrf_PLAT341_s26011m_sq
;
PROBLEM: Low Bond Precision on C-C Bonds ..... 0.01462 Ang.
RESPONSE: ...
;
# end Validation Reply Form
```

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.

