

# checkCIF () running

Checking for embedded fcf data in CIF ...

Found embedded fcf data in CIF. Extracting fcf data from uploaded CIF, please wait . . . . .

## checkCIF/PLATON (full publication check)

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

No syntax errors found.

[CIF dictionary](#)  
[Interpreting this report](#)

[Structure factor report](#)

### Datablock: I

Bond precision:	C-C = 0.0058 Å	Wavelength=0.71073
Cell:	a=13.2478(4)      b=15.6986(4)      c=19.7010(5)	
	alpha=90      beta=90      gamma=90	
Temperature:	140 K	
	Calculated	Reported
Volume	4097.26(19)	4097.25(19)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety	C34 H31 Ag2 N5 P2,	?
formula	2(B F4), C2 H3 N	
Sum formula	C36 H34 Ag2 B2 F8 N6	C36 H34 Ag2 B2 F8 N6
	P2	P2
Mr	1001.99	1001.99
Dx, g cm-3	1.624	1.624
Z	4	4
Mu (mm-1)	1.105	1.105
F000	1992.0	1992.0
F000'	1986.55	
h, k, lmax	18, 21, 26	17, 21, 26
Nref	10901[ 6004]	9167
Tmin, Tmax	0.735, 0.886	0.922, 1.000
Tmin'	0.643	
Correction method=	# Reported T Limits: Tmin=0.922 Tmax=1.000	AbsCorr = MULTI-SCAN
Data completeness=	1.53/0.84	Theta(max)= 29.015
R(reflections)=	0.0260( 8486)	wR2(reflections)= 0.0557( 9167)
S =	1.022	Npar= 555

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

PLAT995\_ALERT\_1\_B Can not Recreate .fcf from Embedded .res & .hkl

! Check

## Alert level C

PLAT048_ALERT_1_C	MoietyFormula Not Given (or Incomplete) .....	Please Check
PLAT220_ALERT_2_C	NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range	4.1 Ratio
PLAT222_ALERT_3_C	NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range	4.8 Ratio
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	N4A Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C21A Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	C31A Check

## Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	10 Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	10 Report
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	1 Info
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	2 Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	1 Report
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Ag1 --N4A .	5.5 s.u.
PLAT244_ALERT_4_G	Low 'Solvent' Ueq as Compared to Neighbors of	B1 Check
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3 )	100% Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 4 )	100% Note
PLAT432_ALERT_2_G	Short Inter X...Y Contact F21 ..C1	2.87 Ang.
	x,y,z =	1_555 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact F22 ..C2	2.92 Ang.
	1/2+x,3/2-y,1-z =	4_566 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact F24 ..C1	2.86 Ang.
	x,y,z =	1_555 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact F32 ..C1	2.83 Ang.
	x,y,z =	1_555 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact F32 ..C41A	2.94 Ang.
	x,y,z =	1_555 Check
PLAT760_ALERT_1_G	CIF Contains no Torsion Angles .....	? Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....	200 Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	1 Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity .....	4.0 Low

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain  
1 **ALERT level B** = A potentially serious problem, consider carefully  
6 **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

- 3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
12 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  
6 ALERT type 4 Improvement, methodology, query or suggestion  
1 ALERT type 5 Informative message, check

## checkCIF publication errors

### Alert level A

PUBL004_ALERT_1_A	The contact author's name and address are missing, _publ_contact_author_name and _publ_contact_author_address.
PUBL005_ALERT_1_A	_publ_contact_author_email, _publ_contact_author_fax and _publ_contact_author_phone are all missing. At least one of these should be present.
PUBL006_ALERT_1_A	_publ_requested_journal is missing e.g. 'Acta Crystallographica Section C'
PUBL008_ALERT_1_A	_publ_section_title is missing. Title of paper.
PUBL009_ALERT_1_A	_publ_author_name is missing. List of author(s) name(s).
PUBL010_ALERT_1_A	_publ_author_address is missing. Author(s) address(es).
PUBL012_ALERT_1_A	_publ_section_abstract is missing. Abstract of paper in English.

### Alert level G

PUBL017_ALERT_1_G	The _publ_section_references section is missing or empty.
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- 7 **ALERT level A** = Data missing that is essential or data in wrong format

### Publication of your CIF

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.

If level A alerts remain, which you believe to be justified deviations, and you intend to submit this CIF for publication in a journal, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. This will allow your explanation to be considered as part of the review process.

### Validation response form

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

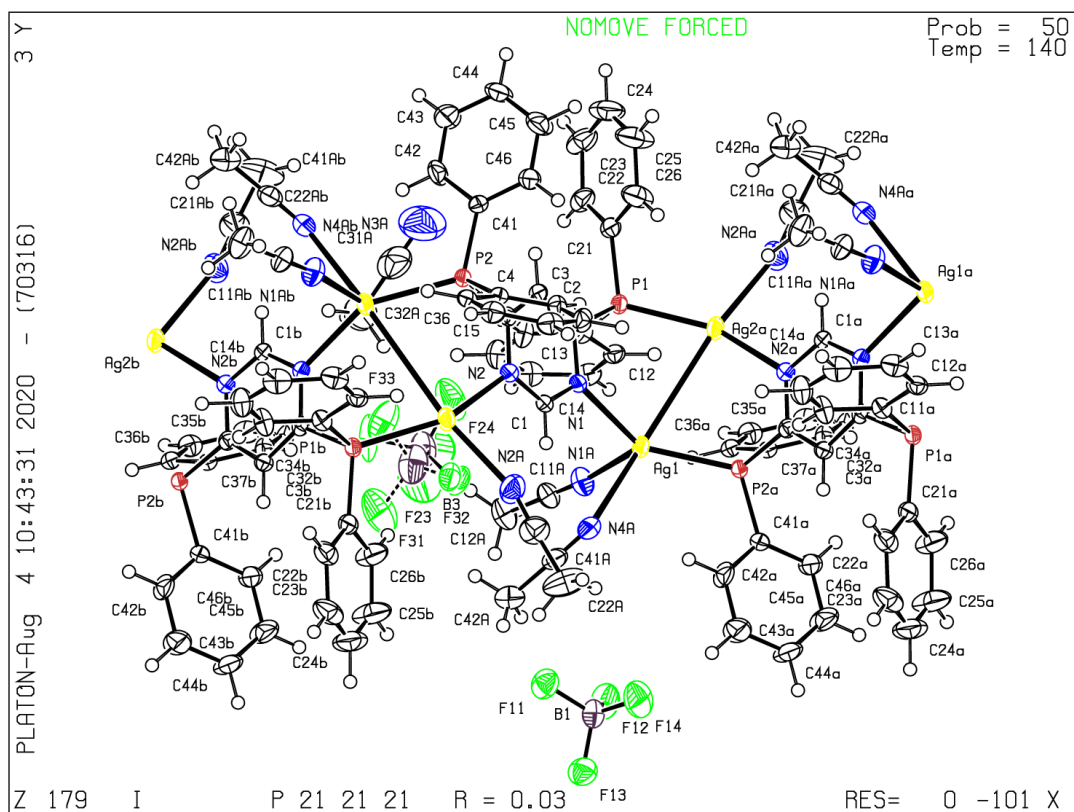
```
# start Validation Reply Form
_vrf_PUBL004_GLOBAL
;
PROBLEM: The contact author's name and address are missing,
RESPONSE: ...
;
_vrf_PUBL005_GLOBAL
;
PROBLEM: _publ_contact_author_email, _publ_contact_author_fax and
RESPONSE: ...
;
_vrf_PUBL006_GLOBAL
;
PROBLEM: _publ_requested_journal is missing
RESPONSE: ...
;
_vrf_PUBL008_GLOBAL
;
PROBLEM: _publ_section_title is missing. Title of paper.
RESPONSE: ...
;
_vrf_PUBL009_GLOBAL
;
PROBLEM: _publ_author_name is missing. List of author(s) name(s).
RESPONSE: ...
;
_vrf_PUBL010_GLOBAL
;
PROBLEM: _publ_author_address is missing. Author(s) address(es).
RESPONSE: ...
;
_vrf_PUBL012_GLOBAL
;
PROBLEM: _publ_section_abstract is missing.
RESPONSE: ...
;
# end Validation Reply Form
```

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via [the web](#). If you wish to submit your CIF for publication in IUCrData you should upload your CIF via [the web](#). If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic [submission](#) or by the Co-editor handling your paper, to upload your CIF via our web site.

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**PLATON version of 16/07/2020; check.def file version of 12/07/2020**

**Datablock I - ellipsoid plot**



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 Download CIF editor (enCIFer) from the CCDC  
 Test a new CIF entry