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 = 0.0090 A              Wavelength=0.71073
Cell:        a=9.2947(2)      b=18.5982(5)     c=18.3144(4)
             alpha=90         beta=90.534(2)   gamma=90
Temperature: 140 K
             Calculated           Reported
Volume       3165.78(13)          3165.78(13)
Space group  P 21/n               P 21/n
Hall group   -P 2yn               -P 2yn
Moiety       C60 H50 Ag2 N8 O6    ?
formula      P4, C2 H3 N
Sum formula  C62 H53 Ag2 N9 O6 P4 C62 H53 Ag2 N9 O6 P4
Mr           1359.76              1359.75
Dx,g cm-3    1.426                1.426
Z            2                    2
Mu (mm-1)    0.776                0.776
F000         1380.0               1380.0
F000'        1377.67
h,k,lmax     12,25,24             12,24,24
Nref         8176                 6793
Tmin,Tmax    0.894,0.933          0.993,1.000
Tmin'        0.850
Correction method= # Reported T Limits: Tmin=0.993 Tmax=1.000 AbsCorr = MULTI-
SCAN
Data completeness= 0.831                  Theta(max)= 28.679
R(reflections)= 0.0634( 5449)     wR2(reflections)= 0.1797( 6793)
S = 1.064        Npar= 565
```

```
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

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☐ 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	3.6 Ratio
PLAT222_ALERT_3_C	NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range	4.4 Ratio
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	Ag1 Check
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds	0.009 Ang.

Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	43 Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	53 Report
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	9.39 Why ?
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	9 Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	7 Report
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Ag1 --P1 .	11.2 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Ag1 --P2_a .	11.7 s.u.
PLAT300_ALERT_4_G	Atom Site Occupancy of N2A Constrained at	0.5 Check

And 5 other PLAT300 Alerts

PLAT300_ALERT_4_G	Atom Site Occupancy of C21A Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C22A Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H22A Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H22B Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H22C Constrained at	0.5 Check
PLAT301_ALERT_3_G	Main Residue Disorder ....(Resd 1)	48% Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)	100% Note
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	13 Note
PLAT760_ALERT_1_G	CIF Contains no Torsion Angles	? Info
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms	! Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	937 Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	11 Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	2.1 Low

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

   3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   8 ALERT type 2 Indicator that the structure model may be wrong or deficient
   5 ALERT type 3 Indicator that the structure quality may be low
  10 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.

```
   7 ALERT level A = Data missing that is essential or data in wrong format
   1 ALERT level G = General alerts. Data that may be required is missing
```

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.
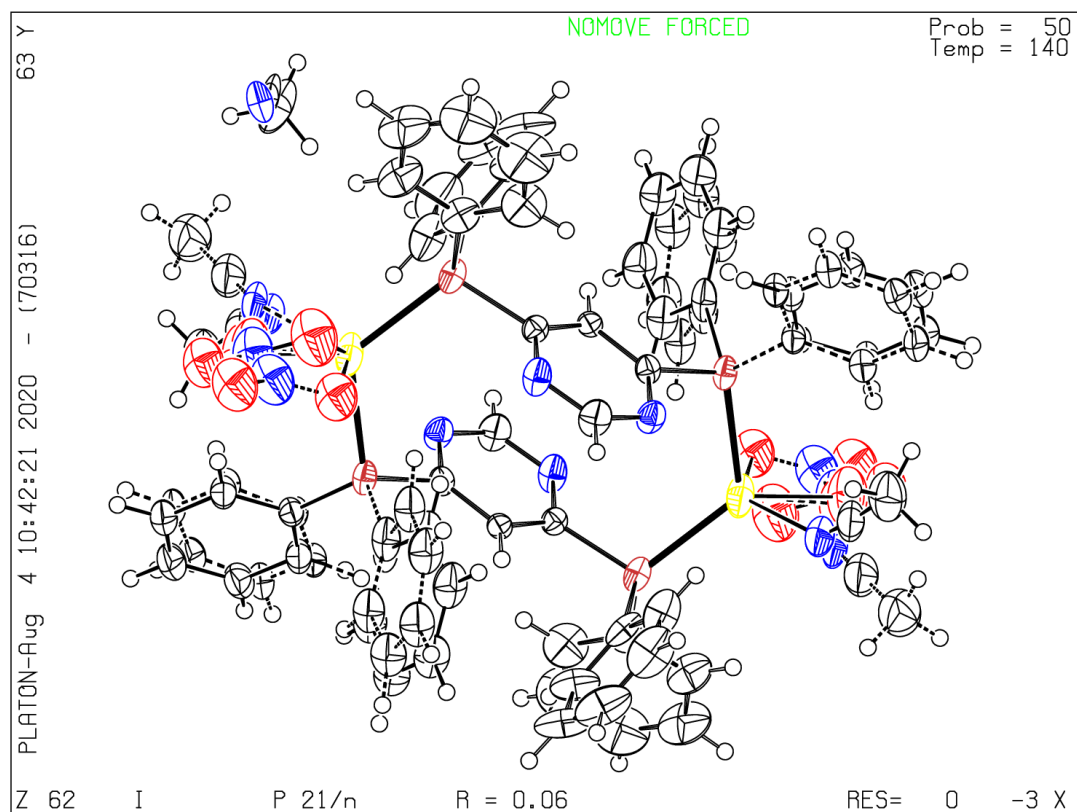
Validation response form

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.

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

Datablock I - ellipsoid plot