checkCIF (full publication check) 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)

Structure factors have been supplied for datablock(s) KSM26_0m_a

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
Please wait while processing .... Interpreting this report

Structure factor report

Datablock: KSM26_0m_a

Bond precision: C-C = 0.0014 A Wavelength=0.71073

Cell: a=9.5722(11) b=15.0133(17) c=21.978(2)
alpha=90 beta=90 gamma=90

Temperature: 150 K

	Calculated	Reported
Volume	3158.5(6)	3158.5(6)
Space group	P b c a	P b c a
Hall group	-P 2ac 2ab	-P 2ac 2ab
Moiety formula	C16 H14 Cl N O4 S	C16 H14 Cl N O4 S
Sum formula	C16 H14 Cl N O4 S	C16 H14 Cl N O4 S
Mr	351.79	351.79
Dx,g cm-3	1.480	1.480
Z	8	8
Mu (mm-1)	0.393	0.393
F000	1456.0	1456.0
F000'	1458.83	
h,k,lmax	14,22,32	14,22,32
Nref	5534	5453
Tmin,Tmax	0.889,0.939	0.890,0.940
Tmin'	0.887	

Correction method= # Reported T Limits: Tmin=0.890 Tmax=0.940 AbsCorr = 'N

Data completeness= 0.985 Theta(max)= 32.100

R(reflections)= 0.0319(4943) wR2(reflections)= 0.0929(5453)

S = 1.069 Npar= 208

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

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 74 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF .... 36 Note

Alert level G

ABSTY01_ALERT_1_G Extra text has been found in the _exptl_absorpt_correction_type field, which should be only a single keyword. A literature citation should be included in the _exptl_absorpt_process_details field.
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check
PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O1 . 109.4 Degree
PLAT480_ALERT_4_G Long H...A H-Bond Reported H2 ..CL1 . 2.84 Ang.

And 2 other PLAT480 Alerts
More ...
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 2 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 4 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 8 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 16 Info

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

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

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checkCIF publication errors

Alert level A
PUBL003_ALERT_1_A The contact author's name is missing,
_publ_contact_author_name.
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'
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).

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5 **ALERT level A** = Data missing that is essential or data in wrong format
0 **ALERT level G** = General alerts. Data that may be required is missing

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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.

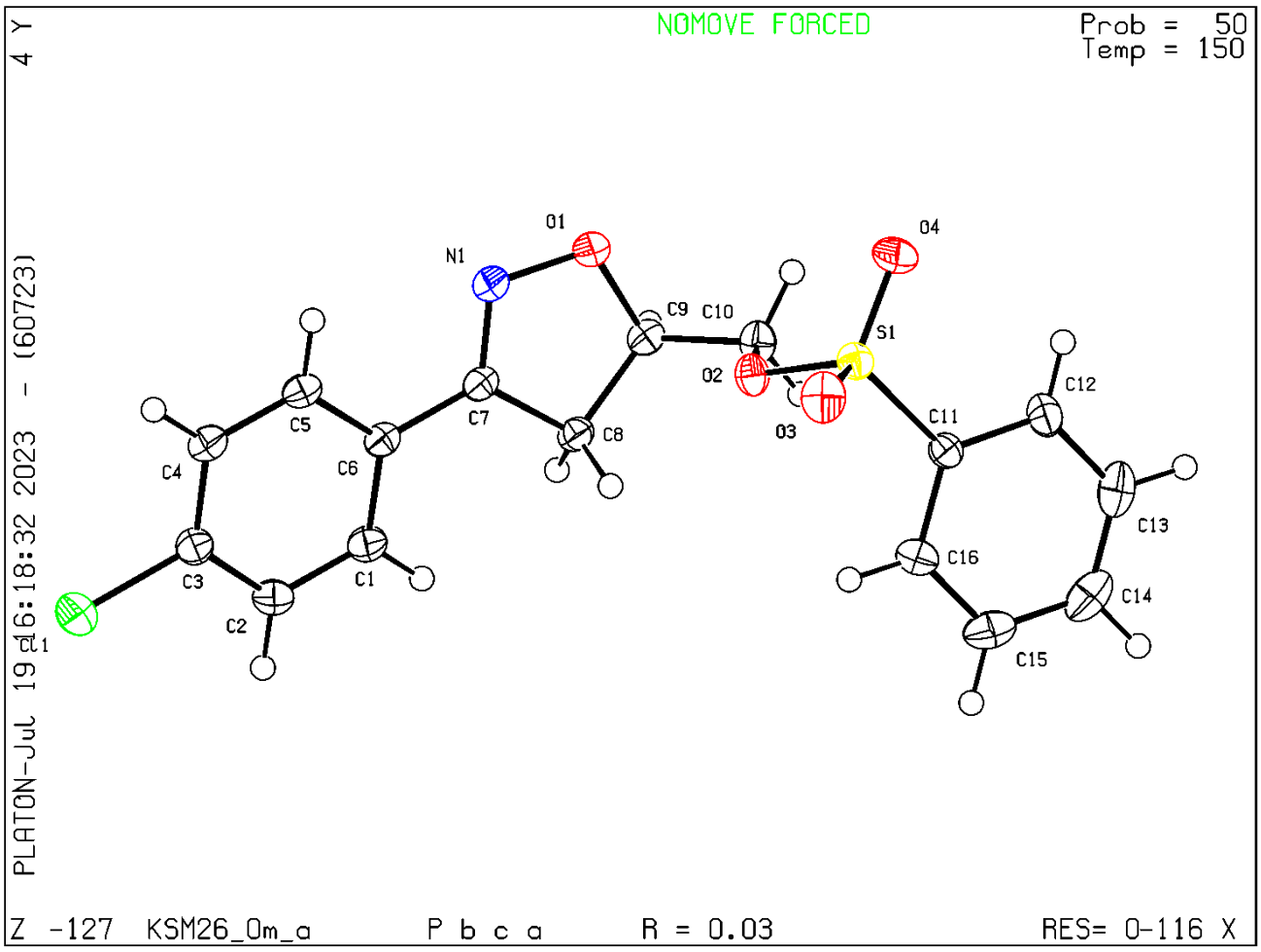
```
# start Validation Reply Form
_vrf_PUBL003_GLOBAL
;
PROBLEM: The contact author's name is missing,
RESPONSE: ...
;
_vrf_PUBL005_GLOBAL
;
PROBLEM: _publ_contact_author_email, _publ_contact_author_fax and
RESPONSE: ...
;
_vrf_PUBL006_GLOBAL
;
PROBLEM: _publ_requested_journal is missing
RESPONSE: ...
;
_vrf_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: ...
;
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 06/07/2023; check.def file version of 30/06/2023

Datablock KSM26_0m_a - ellipsoid plot



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