

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) solve_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 Interpreting this report

Datablock: solve_a

Bond precision:	C-C = 0.0052 A	Wavelength=0.71073	
Cell:	a=11.3946 (16)	b=5.4335 (8)	c=17.977 (3)
	alpha=90	beta=100.055 (6)	gamma=90
Temperature:	293 K		
	Calculated	Reported	
Volume	1095.9 (3)	1095.9 (3)	
Space group	P 21	P 1 21 1	
Hall group	P 2yb	P 2yb	
Moiety formula	C22 H20 O4, O3 S	0.5 (O3 S), 0.5 (C22 H20 O4)	
Sum formula	C22 H20 O7 S	C11 H10 O3.50 S0.50	
Mr	428.44	214.22	
Dx, g cm ⁻³	1.298	1.298	
Z	2	4	
Mu (mm ⁻¹)	0.187	0.187	
F000	448.0	448.0	
F000'	448.50		
h, k, lmax	15, 7, 24	15, 7, 23	
Nref	5459 [3012]	5447	
Tmin, Tmax	0.972, 0.990	0.572, 0.746	
Tmin'	0.943		

Correction method= # Reported T Limits: Tmin=0.572 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.81/1.00 Theta(max)= 28.341

R(reflections)= 0.0580 (4859)	wR2(reflections)=
S = 1.034	0.1619 (5447)
Npar= 275	

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

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75

The relevant atom site should be identified.

STRVA01_ALERT_4_C Flack test results are ambiguous.

From the CIF: `_refine_ls_abs_structure_Flack` 0.480

From the CIF: `_refine_ls_abs_structure_Flack_su` 0.150

PLAT042_ALERT_1_C	Calc. and Reported MoietyFormula Strings Differ	Please Check
PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	2.30 Report
PLAT097_ALERT_2_C	Large Reported Max. (Positive) Residual Density	1.28 eA-3
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	S1 Check
PLAT340_ALERT_3_C	Low Bond Precision on C-C Bonds	0.00523 Ang.
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	2 Report
PLAT976_ALERT_2_C	Check Calcd Resid. Dens. 0.64Ang From O6 .	-0.52 eA-3
PLAT976_ALERT_2_C	Check Calcd Resid. Dens. 0.51Ang From O6 .	-0.51 eA-3
PLAT976_ALERT_2_C	Check Calcd Resid. Dens. 0.62Ang From O7 .	-0.50 eA-3
PLAT976_ALERT_2_C	Check Calcd Resid. Dens. 0.50Ang From O7 .	-0.44 eA-3

Alert level G

PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	2 Report
PLAT033_ALERT_4_G	Flack x Value Deviates > 3.0 * sigma from Zero .	0.480 Note
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.500 Check
PLAT199_ALERT_1_G	Reported <code>_cell_measurement_temperature</code> (K)	293 Check
PLAT200_ALERT_1_G	Reported <code>_diffrn_ambient_temperature</code> (K)	293 Check
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. # O3 S	2 Note
PLAT883_ALERT_1_G	No Info/Value for <code>_atom_sites_solution_primary</code> .	Please Do !
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	3 Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	1 Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	7 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
11 **ALERT level G** = General information/check it is not something unexpected
- 6 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
3 ALERT type 3 Indicator that the structure quality may be low
5 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.

7 **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

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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