

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: 21srv209

Bond precision:	C-C = 0.0057 A	Wavelength=0.71073
Cell:	a=30.1401(10)	b=9.6025(4) c=23.4611(8)
	alpha=90	beta=92.593(1) gamma=90
Temperature:	120 K	
	Calculated	Reported
Volume	6783.2(4)	6783.2(4)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	2(C16 H16 Cl N3 O3 S), H2 O	C16 H16 Cl N3 O3 S, 0.5(H2 O)
Sum formula	C32 H34 Cl2 N6 O7 S2	C32 H34 Cl2 N6 O7 S2
Mr	749.67	374.83
Dx,g cm-3	1.468	1.468
Z	8	16
Mu (mm-1)	0.372	0.372
F000	3120.0	3120.0
F000'	3125.60	
h,k,lmax	41,13,32	41,13,32
Nref	18018	18001
Tmin,Tmax	0.948,0.982	0.349,0.494
Tmin'	0.881	

Correction method= # Reported T Limits: Tmin=0.349 Tmax=0.494
AbsCorr = MULTI-SCAN

Data completeness= 0.999 Theta(max)= 29.000

R(reflections)= 0.0842(12598) wR2(reflections)= 0.2080(18001)

S = 1.127 Npar= 979

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 A

ABSMU01_ALERT_1_A The ratio of given/expected absorption coefficient lies outside the range 0.90 <> 1.10

Calculated value of mu = 0.744

Value of mu given = 0.372

CHEMW01_ALERT_1_A The ratio of given/expected molecular weight as calculated from the _chemical_formula_sum lies outside the range 0.90 <> 1.10

Calculated formula weight = 749.6826

Formula weight given = 374.8300

PLAT010_ALERT_1_A No Suitable (Embedded) Reflection Data Supplied Please Do !

Alert level B

PLAT008_ALERT_5_B No _iucr_refine_reflections_details in the CIF Please Do !

PLAT417_ALERT_2_B Short Inter D-H..H-D H3BA ..H2WB . 2.00 Ang.

x,y,z = 1_555 Check

PLAT995_ALERT_1_B Can not Recreate .fcf from Embedded .res & .hkl ! Check

Alert level C

CHEMW01_ALERT_1_C The difference between the given and expected weight for compound is greater 1 mass unit. Check that all hydrogen atoms have been taken into account.

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check

PLAT222_ALERT_3_C NonSolvent Resd 4 H Uiso(max)/Uiso(min) Range 4.7 Ratio

PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds 0.00573 Ang.

PLAT353_ALERT_3_C Long N-H (N0.87,N1.01A) N3 - H3A . 1.01 Ang.

PLAT353_ALERT_3_C Long N-H (N0.87,N1.01A) N3A - H3AB . 1.02 Ang.

PLAT353_ALERT_3_C Long N-H (N0.87,N1.01A) N3B - H3BB . 1.01 Ang.

PLAT353_ALERT_3_C Long N-H (N0.87,N1.01A) N3C - H3CA . 1.01 Ang.

PLAT420_ALERT_2_C D-H Bond Without Acceptor N3A --H3AB . Please Check

Alert level G

FORMU01_ALERT_1_G There is a discrepancy between the atom counts in the _chemical_formula_sum and _chemical_formula_moiety. This is usually due to the moiety formula being in the wrong format.

Atom count from _chemical_formula_sum: C32 H34 Cl2 N6 O7 S2

Atom count from _chemical_formula_moiety: C16 H17 Cl1 N3 O3.5 S1

FORMU01_ALERT_2_G There is a discrepancy between the atom counts in the _chemical_formula_sum and the formula from the _atom_site* data.

Atom count from _chemical_formula_sum: C32 H34 Cl2 N6 O7 S2

Atom count from the _atom_site data: C16 H17 Cl1 N3 O3.5 S1

CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.

CELLZ01_ALERT_1_G ALERT: Large difference may be due to a

symmetry error - see SYMMG tests

From the CIF: _cell_formula_units_Z 16

From the CIF: _chemical_formula_sum C32 H34 Cl2 N6 O7 S2

TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	512.00	256.00	256.00
H	544.00	272.00	272.00
Cl	32.00	16.00	16.00
N	96.00	48.00	48.00

O	112.00	56.00	56.00	
S	32.00	16.00	16.00	
PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite			26 Note
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms			2 Report
PLAT012_ALERT_1_G	No	_shelx_res_checksum	Found in CIF	Please Check
PLAT042_ALERT_1_G	Calc. and Reported Moiety Formula Strings Differ			Please Check
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...			0.50 Check
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large			24.95 Why ?
PLAT112_ALERT_2_G	ADDSYM	Detects New (Pseudo) Symm. Elem	sub	93 %Fit
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records			1 Report
PLAT173_ALERT_4_G	The CIF-Embedded .res File Contains DANG Records			2 Report
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records			4 Report
PLAT431_ALERT_2_G	Short Inter HL..A Contact	C11	..03A	3.15 Ang.
		1-x,1-y,1-z =		3_666 Check
PLAT431_ALERT_2_G	Short Inter HL..A Contact	C11C	..02B	3.14 Ang.
		x,1/2-y,-1/2+z =		4_565 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	O1	..C11B	2.99 Ang.
		1-x,1/2+y,1/2-z =		2_655 Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels			18 Note
PLAT793_ALERT_4_G	Model has Chirality at C1	(Centro SPGR)		S Verify
PLAT793_ALERT_4_G	Model has Chirality at C1A	(Centro SPGR)		R Verify
PLAT793_ALERT_4_G	Model has Chirality at C1B	(Centro SPGR)		S Verify
PLAT793_ALERT_4_G	Model has Chirality at C1C	(Centro SPGR)		R Verify
PLAT860_ALERT_3_G	Number of Least-Squares Restraints			61 Note

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

12 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 9 ALERT type 2 Indicator that the structure model may be wrong or deficient
 7 ALERT type 3 Indicator that the structure quality may be low
 8 ALERT type 4 Improvement, methodology, query or suggestion
 2 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.

```
# 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: ...
;
_vrf_ABSMU01_21srv209
;
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PROBLEM: The ratio of given/expected absorption coefficient lies
RESPONSE: ...
;
_vrf_CHEMW01_21srv209
;
PROBLEM: The ratio of given/expected molecular weight as calculated
RESPONSE: ...
;
_vrf_PLAT010_21srv209
;
PROBLEM: No Suitable (Embedded) Reflection Data Supplied      Please Do !
RESPONSE: ...
;
# end Validation Reply Form

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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 16/05/2021; check.def file version of 13/05/2021

Datablock 21srv209 - ellipsoid plot

