
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 G

PLAT899_ALERT_4_G SHELXL2018 is Deprecated and Succeeded by SHELXL	2019/3 Note
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities	Please Check
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res ..	56.0 Degree
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.	3 Info

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

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
1 ALERT type 2 Indicator that the structure model may be wrong or deficient
0 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check

Datablock: compound-2-primeprime

Bond precision: C-C = 0.0018 A

Wavelength=0.71073

Cell:	a=8.4988(8)	b=17.5628(15)	c=11.3833(11)
	alpha=90	beta=101.860(7)	gamma=90
Temperature:	200 K		

	Calculated	Reported
Volume	1662.8(3)	1662.8(3)
Space group	C 2/c	C 2/c
Hall group	-C 2yc	-C 2yc
Moiety formula	C10 H8 Cl4 N8 Si	C10 H8 Cl4 N8 Si
Sum formula	C10 H8 Cl4 N8 Si	C10 H8 Cl4 N8 Si
Mr	410.13	410.13
Dx, g cm ⁻³	1.638	1.638
Z	4	4
Mu (mm ⁻¹)	0.794	0.794
F000	824.0	824.0
F000'	826.83	
h,k,lmax	12,26,16	12,26,16
Nref	2897	2896
Tmin,Tmax	0.842,0.909	0.859,0.936
Tmin'	0.840	

Datablock: compound-1,5-3

	Calculated	Reported
Volume	1044.43(6)	1044.42(6)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C13 H10 N4	C13 H10 N4
Sum formula	C13 H10 N4	C13 H10 N4
Mr	222.25	222.25
Dx, g cm ⁻³	1.413	1.413
Z	4	4
Mu (mm ⁻¹)	0.090	0.090
F000	464.0	464.0
F000'	464.14	
h, k, lmax	12, 15, 12	12, 15, 12
Nref	2508	2508
Tmin, Tmax	0.963, 0.973	
Tmin'	0.947	

Correction method= Not given

Data completeness= 1.000

Theta(max)= 27.989

R(reflections)= 0.0374(2271)

wR2(reflections)=
0.0922(2508)

S = 1.075

Npar= 155

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

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 2.232 Check



Alert level G

PLAT899_ALERT_4_G SHELXL2018 is Deprecated and Succeeded by SHELXL 2019/3 Note
 PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF 1 Note
 PLAT961_ALERT_5_G Dataset Contains no Negative Intensities Please Check
 PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res .. 56.0 Degree
 PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 14 Info

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

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

1 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check

Datablock: compound-1,4-3

Bond precision: C-C = 0.0030 Å

Wavelength=0.71073

Cell: a=5.6770(4) b=7.1648(5) c=13.4102(11)
alpha=75.071(6) beta=79.636(6) gamma=89.686(6)
Temperature: 180 K

	Calculated	Reported
Volume	517.96(7)	517.96(7)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C13 H10 N4	C13 H10 N4
Sum formula	C13 H10 N4	C13 H10 N4
Mr	222.25	222.25
Dx, g cm ⁻³	1.425	1.425
Z	2	2
Mu (mm ⁻¹)	0.090	0.090
F000	232.0	232.0
F000'	232.07	
h, k, lmax	7, 8, 16	7, 8, 16
Nref	2019	7244
Tmin, Tmax	0.994, 0.996	
Tmin'	0.914	

Correction method= Not given

Data completeness= 3.588

Theta(max)= 25.989

R(reflections)= 0.0488(5459)

wR2(reflections)=
0.1323(7244)

S = 1.052

Npar= 156

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

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 2.635 Check

 **Alert level G**

PLAT063_ALERT_4_G Crystal Size Possibly too Large for Beam Size .. 1.00 mm
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.006 Degree
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed .. ! Info
PLAT899_ALERT_4_G SHELXL2018 is Deprecated and Succeeded by SHELXL 2019/3 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 1 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF 1 Note
PLAT931_ALERT_5_G CIFcalcFCF Twin Law [1 0 0] Est.d BASF 0.38 Check
PLAT931_ALERT_5_G CIFcalcFCF Twin Law [1 0 0] Est.d BASF 0.38 Check
PLAT931_ALERT_5_G CIFcalcFCF Twin Law [1 0 0] Est.d BASF 0.38 Check
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 3.6 Low
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities Please Check
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res .. 52.0 Degree

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
0 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
5 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 06/07/2023; check.def file version of 30/06/2023

Datablock compound-2-prime - ellipsoid plot







